



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 01:42 pm BST

PDB ID : 3I4N
Title : 8-oxoguanine containing RNA polymerase II elongation complex E
Authors : Damsma, G.E.; Cramer, P.
Deposited on : 2009-07-02
Resolution : 3.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

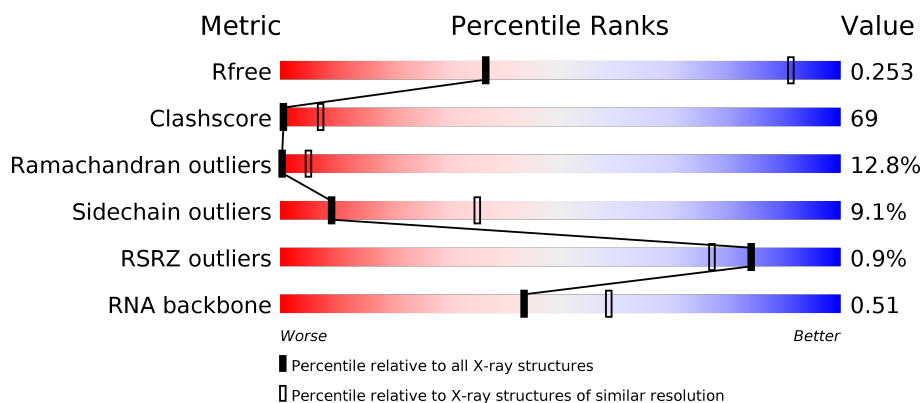
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)
RNA backbone	3102	1040 (4.76-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	<div> <div>17%</div> <div>52%</div> <div>12%</div> <div>•</div> <div>18%</div> </div>
2	B	1224	<div> <div>21%</div> <div>56%</div> <div>13%</div> <div>•</div> <div>8%</div> </div>
3	C	324	<div> <div>19%</div> <div>52%</div> <div>12%</div> <div>•</div> <div>17%</div> </div>
4	D	221	<div> <div>19%</div> <div>48%</div> <div>14%</div> <div>•</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	T	26	
14	N	12	
15	P	16	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32307 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1429	Total	C	N	O	S	0	0	0
			11240	7079	1966	2133	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1125	Total	C	N	O	S	0	0	0
			8942	5659	1571	1657	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	270	Total	C	N	O	S	0	0	0
			2125	1336	353	422	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	EXPRESSION TAG	UNP P16370
C	-4	HIS	-	EXPRESSION TAG	UNP P16370
C	-3	HIS	-	EXPRESSION TAG	UNP P16370
C	-2	HIS	-	EXPRESSION TAG	UNP P16370
C	-1	HIS	-	EXPRESSION TAG	UNP P16370
C	0	HIS	-	EXPRESSION TAG	UNP P16370

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	182	Total	C	N	O	S	0	0	0
			1465	904	262	296	3			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	88	Total	C	N	O	S	0	0	0
			712	455	120	134	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	137	Total	C	N	O	S	0	0	0
			1101	693	185	218	5			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	117	Total	C	N	O	S	0	0	0
			952	586	173	182	11			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	116	Total	C	N	O	S	0	0	0
			929	596	158	173	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	47	Total	C	N	O	S	0	0	0
			370	228	73	65	4			

- Molecule 13 is a DNA chain called DNA (5'-D(*AP*G*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP*(8OG)P*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	T	20	Total	Br	C	N	O	P	0	0	0
			407	1	194	72	121	19			

- Molecule 14 is a DNA chain called DNA (5'-D(*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	11	Total	C	N	O	P	0	0	0
			224	108	42	64	10			

- Molecule 15 is a RNA chain called RNA (5'-R(*UP*GP*CP*AP*UP*C*UP*UP*CP*CP*AP*GP*GP*CP*AP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	10	Total	C	N	O	P	0	0	0
			207	94	35	69	9			

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	J	1	Total	Zn	0	0
			1	1		
17	B	1	Total	Zn	0	0
			1	1		
17	I	2	Total	Zn	0	0
			2	2		
17	C	1	Total	Zn	0	0
			1	1		

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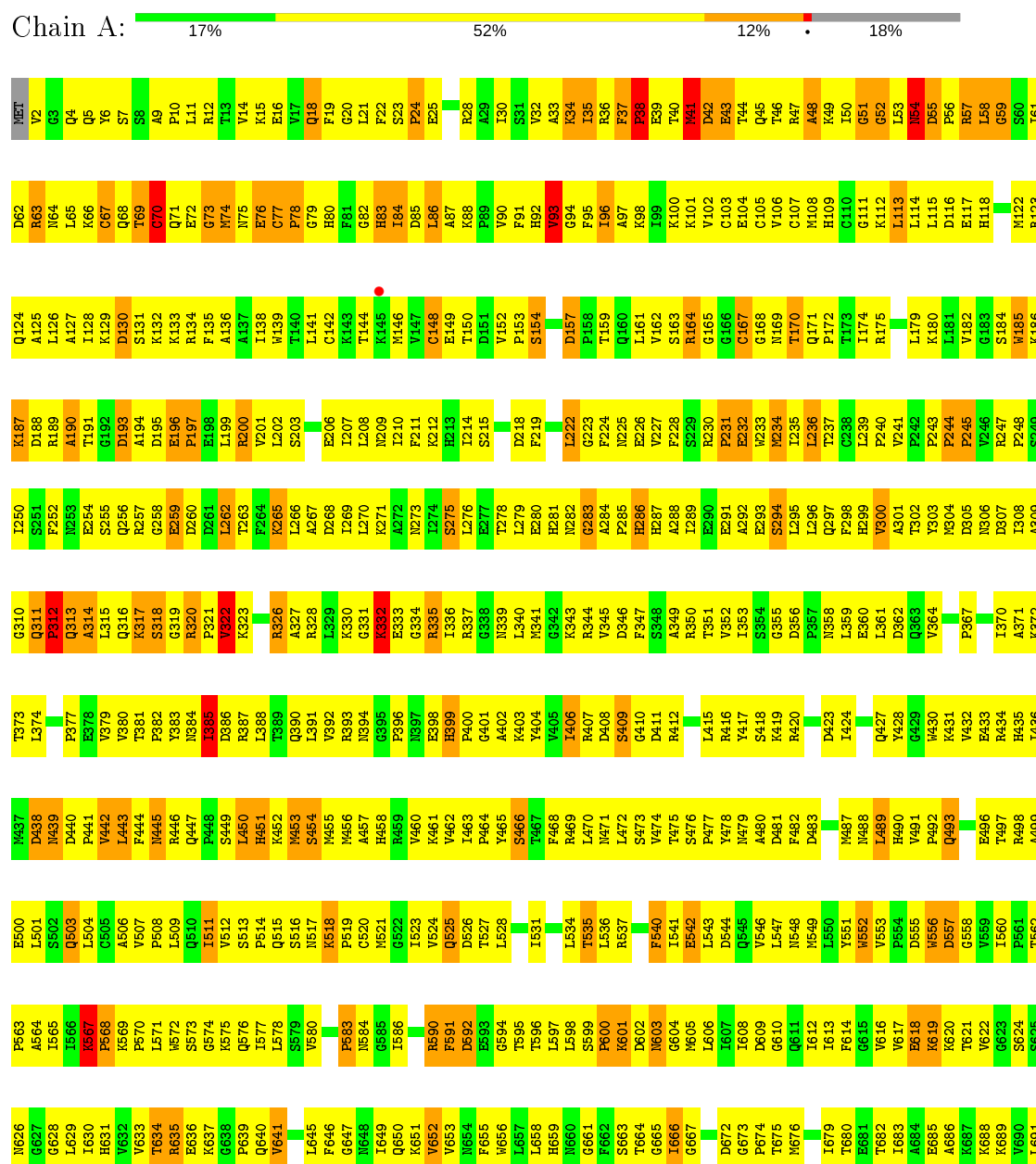
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	2	Total 2	Zn 2	0	0
17	L	1	Total 1	Zn 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



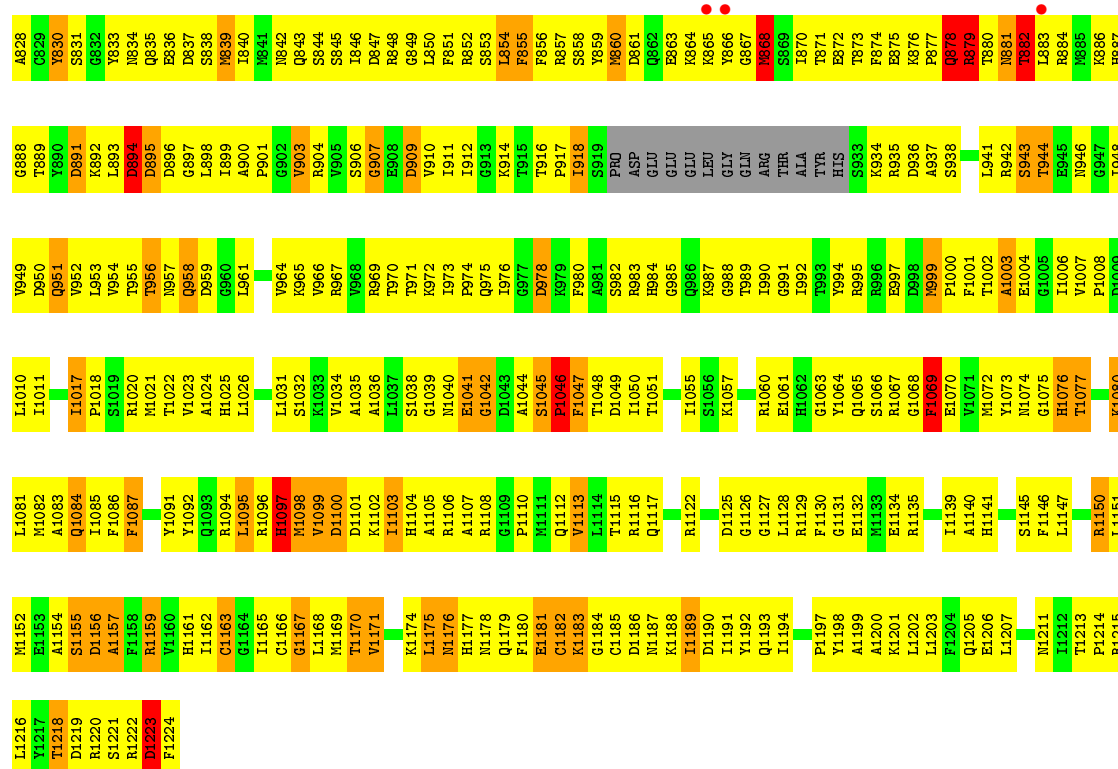
SER	THR	PRO	GLY	K1452	K1453	P1454	P1455	V1319	E1256	L1192	L1193	L1133	L1134	G1070	A1010	L943	H877	H816	G753	D892
THR	SER	THR	GLY	Y1453	Y1454	Y1455	Y1456	D1323	D1257	L1197	L1198	L1133	L1134	S1071	Q1011	R944	I878	A817	S754	V693
PRO	PRO	PRO	ASP	P1454	P1455	P1456	P1457	P1324	H1258	L1197	L1198	L1133	L1134	G1073	D1012	E945	K880	M818	F755	K695
THR	SER	THR	TYR	G1395	G1396	G1397	G1398	T1325	L1260	D1198	D1199	S1136	S1137	P1075	A1014	F947	L863	G820	N757	E996
PRO	SER	PRO	GLU	L1397	L1398	L1399	L1400	R1326	K1261	A1201	M1202	L1137	L1138	P1076	T1016	V948	D884	R821	I758	A697
THR	THR	THR	ILE	Y1328	Y1329	Y1330	Y1331	Y1327	K1262	M1202	M1203	L1138	L1139	A1076	T1017	D949	T885	E822	A759	Q698
THR	THR	THR	THR	T1329	T1330	T1331	T1332	T1328	E1264	M1203	M1204	L1139	L1140	G950	F1018	G951	E951	I825	A699	M700
PRO	SER	PRO	GLU	M1399	M1400	M1401	M1402	M1398	M1265	D1204	D1205	L1141	L1142	Q1078	F1019	E952	G887	D826	S762	L701
PRO	PRO	PRO	ILE	S1401	S1402	S1403	S1404	S1400	T1266	K1205	K1206	T1141	T1142	T1080	C1020	N953	G888	T827	A763	L702
THR	SER	THR	GLU	F1402	F1403	F1404	F1405	F1401	M1267	D1206	D1207	L1143	L1144	T1081	L1021	N954	S869	A828	G764	T703
SER	GLY	ASP	ASP	E1403	E1404	E1405	E1406	E1402	L1268	L1207	L1208	L1144	L1145	ASN	L1022	P955	D890	V829	V765	A704
PRO	SER	PRO	GLY	E1404	E1405	E1406	E1407	E1403	E1269	T1207	T1208	L1144	L1145	THR	E1023	P955	D890	K830	G766	K705
THR	THR	THR	GLN	T1405	T1406	T1407	T1408	T1404	I1270	M1209	M1210	V1146	V1147	PHE	S1024	V958	F893	T831	Q767	H706
PRO	GLY	GLY	ASP	V1405	V1406	V1407	V1408	V1404	I1271	G1210	G1211	H1147	H1148	HIS	R1025	N959	E894	R1025	Q768	G707
PRO	GLY	GLY	GLY	E1407	E1408	E1409	E1410	E1405	T1272	G1211	G1212	L1148	L1149	PHE	L1026	E961	K895	E833	E711	G708
PRO	VAL	VAL	THR	I1408	I1409	I1410	I1411	I1406	L1273	G1213	G1214	L1149	L1150	ALA	A1027	R962	R896	T834	K773	T709
THR	THR	THR	THR	L1409	L1410	L1411	L1412	L1407	G1274	G1213	G1214	S1150	S1151	GLY	T1028	R962	R897	G835	K772	L710
PRO	SER	PRO	PRO	A1412	A1413	A1414	A1415	A1410	G1275	R1214	R1215	E1151	E1152	VAL	R1029	R963	R898	Y836	R771	R711
PRO	SER	PRO	PRO	G1413	G1414	G1415	G1416	G1411	T1276	R1215	R1216	E1152	E1153	ALA	R1030	R964	R899	I837	E712	E712
THR	THR	THR	GLY	A1414	A1415	A1416	A1417	A1412	E1277	I1216	I1217	Y1153	Y1154	SER	V1031	Q965	S713	Q838	S713	S713
PRO	GLY	GLY	ASN	S1415	S1416	S1417	S1418	S1413	N1278	K1217	K1218	Y1154	Y1155	LVS	L1032	N966	L901	R839	A776	F714
PRO	GLY	GLY	ASN	S1415	S1416	S1417	S1418	S1413	I1279	Q1218	Q1219	D1155	D1156	LVS	Q1033	A967	L902	R840	F777	E715
THR	VAL	VAL	SER	E1417	E1418	E1419	E1420	E1415	E1280	T1219	T1220	P1156	P1157	K1093	Q1034	Q968	N903	L841	G778	E716
SER	GLY	GLY	GLY	E1418	E1419	E1420	E1421	E1416	M1284	K1221	K1222	P1158	P1159	S1096	R1035	Q969	T904	V842	F779	N717
THR	GLY	GLY	GLY	E1419	E1420	E1421	E1422	E1417	M1285	K1222	K1223	R1159	R1160	S1097	R1036	T970	L908	R843	V718	V718
PRO	VAL	VAL	VAL	E1420	E1421	E1422	E1423	E1418	E1351	D1223	D1224	S1160	S1161	V1098	L1037	F971	L908	A844	D781	V719
TYR	ALA	ALA	ALA	E1421	E1422	E1423	E1424	E1419	E1352	L1224	L1225	T1161	T1162	P1099	T1038	H972	P910	E846	H782	F721
SER	PHE	PHE	PHE	R1422	R1423	R1424	R1425	R1420	V1352	L1225	L1226	V1162	V1163	R1100	Q1040	I973	P910	D847	L784	L722
PRO	ASP	ASP	ASP	G1423	G1424	G1425	G1426	G1421	V1355	V1226	V1227	L1163	L1164	L1101	A1041	T976	L913	I848	P785	
PRO	LEU	LEU	LEU	V1424	V1425	V1426	V1427	V1422	I1356	I1227	I1228	L1163	L1164	L1102	F1042	R977	E914	M849	H786	
THR	ASP	ASP	ASP	S1425	S1426	S1427	S1428	S1423	D1359	M1228	M1229	E1165	E1166	E1103	D1043	P978	S915	V850	F787	
PRO	VAL	VAL	VAL	E1426	E1427	E1428	E1429	E1424	P1294	D1229	D1230	D1166	D1167	L1104	W1044	S979	R851	R851	S788	D727
PRO	LVS	LVS	LVS	M1427	M1428	M1429	M1430	M1425	G1360	E1230	E1231	E1167	E1168	D980	D1045	D981	S917	Y852	K728	K728
THR	ASP	ASP	ASP	V1428	V1429	V1430	V1431	V1426	S1361	D1231	D1232	E1168	E1169	M1106	L1046	L981	E918	A729	A729	
GLY	GLY	GLY	GLY	I1429	I1430	I1431	I1432	I1427	Y1362	N1232	N1233	T1169	T1170	V1107	S1047	T982	I919	M854	D730	G730
PRO	LEU	LEU	LEU	E1430	E1431	E1432	E1433	E1428	V1363	D1233	D1234	Q1171	Q1172	E1050	M1048	R983	L920	T856	P794	
THR	PHE	PHE	PHE	Q1431	Q1432	Q1433	Q1434	Q1429	M1364	L1236	L1237	M1111	M1112	E1051	I1049	K984	D921	T856	E795	
PRO	PRO	PRO	PRO	E1432	E1433	E1434	E1435	E1430	Y1365	L1237	L1238	K1112	K1113	Q1052	E1052	D985	D922	R857	S796	L732
PRO	PRO	PRO	PRO	M1433	M1434	M1435	M1436	M1431	R1366	I1238	I1239	F1173	F1174	F1053	Q1053	I986	L923	M858	E734	E734
THR	ALA	ALA	ALA	P1435	P1436	P1437	P1438	P1433	M1367	R1239	R1240	S1175	S1176	P1054	L1054	L993	K924	S859	V735	V735
SER	VAL	VAL	VAL	I1436	I1437	I1438	I1439	I1434	A1368	G1240	G1241	L1175	L1176	R1055	Q926	Q994	Q926	L860	L737	L737
PRO	ASP	ASP	ASP	G1437	G1438	G1439	G1440	G1435	L1370	R1241	R1242	S1176	S1177	R1055	V927	N995	N927	G861	V800	
THR	GLY	GLY	GLY	T1438	T1439	T1440	T1441	T1436	W1304	V1242	V1243	D1178	D1179	S1056	V863	N996	L928	N862	E801	K738
SER	GLY	GLY	GLY	G1439	G1440	G1441	G1442	G1437	L1306	V1243	V1244	E1179	E1180	V1057	I864	L997	L929	I864	N802	D739
PRO	ASN	ASN	ASN	A1440	A1441	A1442	A1443	A1438	E1307	R1244	R1245	GLU	GLU	V1058	Q865	L998	D930	Q865	Y804	L740
THR	ASP	ASP	ASP	F1441	F1442	F1443	F1444	F1439	T1308	P1245	P1246	ALA	ALA	H1059	F866	V999	E931	F866	M742	M742
PRO	ALA	ALA	ALA	D1442	D1443	D1444	D1445	D1440	D1309	K1246	K1247	GLU	GLU	P1060	I867	L1000	E932	I867	R806	V743
SER	THR	THR	THR	E1443	E1444	E1445	E1446	E1441	G1310	SER	SER	GLN	GLN	G1061	Y868	K1001	Y933	Y868	G807	K743
PRO	MET	MET	MET	V1443	V1444	V1445	V1446	V1441	V1311	LEU	LEU	GLN	GLN	E1062	G1002	G1003	Y933	G869	L808	Q745
THR	ALA	ALA	ALA	Q1378	Q1379	Q1380	Q1381	Q1376	M1312	ASP	ASP	PHE	PHE	M1063	K1003	K1004	L936	E870	M746	M746
TYR	GLY	GLY	GLY	G1379	G1380	G1381	G1382	G1377	L1313	ALA	ALA	ASP	ASP	M1064	N1004	N1005	V937	D871	P810	V747
PRO	GLY	GLY	GLY	E1447	E1448	E1449	E1450	E1444	S1383	GLU	GLU	O1187	O1188	G1065	G1066	I005	K938	Q811	M748	
PRO	PHE	PHE	PHE	E1448	E1449	E1450	E1451	E1444	E1315	THR	THR	Q1188	Q1189	V1066	I1006	I1007	D939	M873	E812	A749
THR	THR	THR	THR	S1449	S1450	S1451	S1452	S1444	V1316	GLU	GLU	Q1189	Q1190	L1067	I1007	I1008	R940	D874	F813	
SER	ALA	ALA	ALA	M1317	M1318	M1319	M1320	M1314	M1315	E1254	E1255	E1189	E1190	L1067	K941	Q1008	K940	A875	S751	
PRO	TYR	TYR	TYR	V1451	V1452	V1453	V1454	V1449	N1390	E1255	E1256	W1191	W1192	Q1130	A1069	N1009	F942	A876	F815	F752

THR	SER	PRO	ASN	TRP	SER	PRO	THR	THR	PRO	SER	TRP	SER	PRO	THR	THR	PRO	THR	GLY	PRO	GLY	THR	THR	GLU	SER	PRO	GLY	GLN	GLN	LYS	HIS	ASN	GLU	ASN	ASN	ARG
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● Molecule 2: DNA-directed RNA polymerase II subunit RPB2

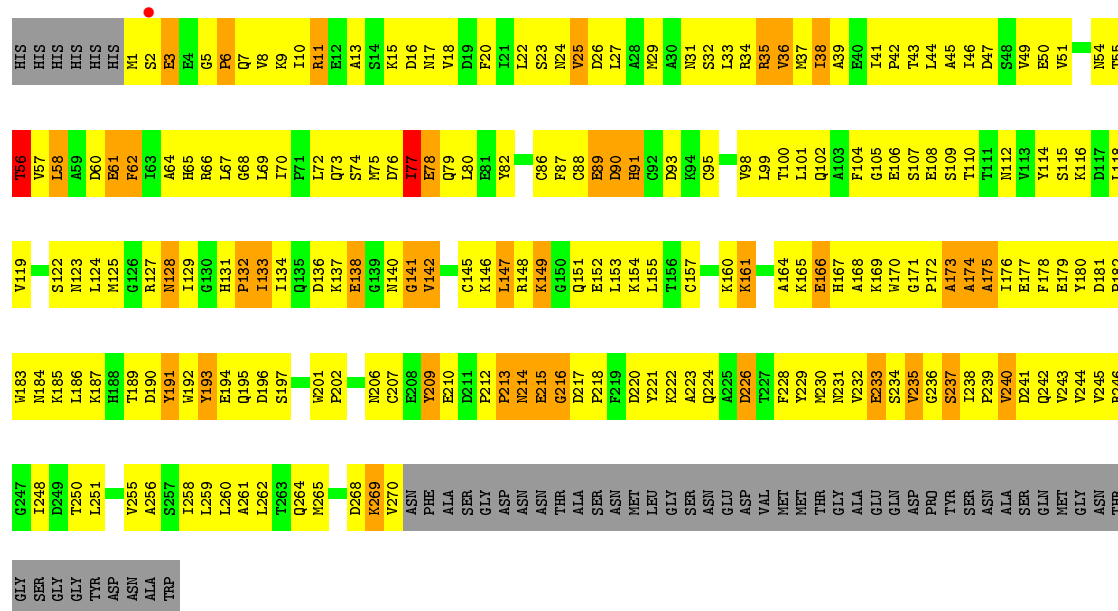


MET	SER	ASP	LEU	ALA	ASN	SER	GLU	LYS	TRP	ASP	GLU	ASP	PRO	TRP	THR	GLY	PHE	GLU	THR	GLU	SER	D20	E21	S22	A23	P24	I25	T26	D29	S30	L31	S32	F33	I34	S35	A36	V37	F38	R39	K40	G42	L43	V44	S45	Q46	Q47	L48	D49	S50	F51	N52	Q53	F54	V55	D56	Y57	T58	L59	Q60	S125	
I62	I63	C64	E65	D66	V67	T68	L69	I70	LEU	GLN	LEU	ALA	GLN	PRO	THR	THR	THR	THR	THR	THR	GLU	SER	D20	E21	S22	A23	P24	I25	T26	D29	S30	L31	S32	F33	I34	S35	A36	V37	F38	R39	K40	G42	L43	V44	S45	Q46	Q47	L48	D49	S50	F51	N52	Q53	F54	V55	D56	Y57	T58	L59	Q60	S125
S126	G127	F128	F129	D130	D131	V132	K133	K134	R135	E136	ALA	ILE	ASP	VAL	PRO	GLY	ARG	GLU	GLU	SER	D20	E21	S22	A23	P24	I25	T26	D29	S30	L31	S32	F33	I34	S35	A36	V37	F38	R39	K40	G42	L43	V44	S45	Q46	Q47	L48	D49	S50	F51	N52	Q53	F54	V55	D56	Y57	T58	L59	Q60	S125		
S187	D188	L189	Y190	K191	L192	K193	E194	C195	P196	F197	Y202	F203	I204	I205	N206	G207	K210	V211	L212	I213	A214	Q215	E216	R217	S218	A219	G220	N221	I222	V223	Q224	K227	K228	A229	A230	P231	I234	S235	H236	V237	A238	M239	R240	R241	R242	A243	L244	G247	S248	R249	F250	L251	E183	A184	T185	E186					
L254	Q255	V256	K257	L258	Y259	G260	R261	S265	A266	R267	T268	I269	K270	A271	T272	L273	P274	P275	I276	K277	Q278	D279	I280	Q281	I282	V283	I284	G285	R286	R287	A288	G290	I291	I292	P293	D294	E296	I297	L298	E299	H300	Y303	D304	V305	N306	D307	W308	Q309	R310	L311	L312	K313	L314	K315	P316						
C317	V318	E319	D320	V323	I324	Q325	R326	R327	C328	T329	A330	L331	D332	F333	I334	G335	R336	R337	G338	T339	A340	L341	G342	I343	K344	K345	E346	K347	R348	I349	Q350	Y351	A352	K353	D354	L355	Q357	K358	E359	F360	L361	P362	H363	T364	Q365	L367	E368	G369	F370	E371	K372	R373	K374	A375	F376	F377					
L378	G379	S380	N381	I382	K383	R384	L385	L386	L387	C388	A389	L390	D391	R392	K393	D394	Q395	D396	F401	G402	K403	K404	B405	L406	P407	L408	A409	G410	P411	L412	L413	A414	Q415	L416	F417	K418	F419	L420	F421	K422	K423	L424	T425	F429	R430	R434	T435	V436	E437	GLU	ALA	HIS	ASP	PHE	ASN	MET					
LYS	L446	A447	L448	A449	A450	K451	F452	L453	T454	S455	A456	L457	K458	A459	A460	L461	D464	N465	N466	G467	E468	Q469	K470	K471	A472	L473	S474	G475	K476	A477	L478	P479	S480	Q481	V482	L483	N484	R485	Y486	T487	Y488	S489	S490	T491	L492	L495	R496	R497	T498	Y499	T500	P501	P502	G503	H504	P505	G506				
K507	L508	A509	K510	P511	R512	Q513	L514	M515	N516	T517	G518	H519	H520	L521	A525	E526	T527	P528	E529	G530	Q531	V536	K537	N538	M542	S543	S546	V547	G548	T549	D550	L555	T556	F557	L558	S559	E560	V561	G562	M563	K564	P565	F566	T567	D568	E569	V570	P571	H572	Q573	S574	P575	D576	A577							
T578	R579	V580	F581	N582	V583	G584	S585	M586	H587	G588	V589	H590	H591	H592	A593	A594	R595	L596	M597	E598	T599	L600	B601	T602	L603	R604	R605	G606	G607	T608	M609	M610	E611	E612	V613	S614	N615	I616	R617	D618	I619	R620	E621	E622	K625	I626	F627	T628	D629	A630	G631	R632	R633	V634	R635	P636	L637	F638			
I639	V640	E641	D642	D643	H648	K649	E650	L651	K652	G653	V654	R655	H656	H657	I658	A659	K660	L661	M662	A663	T664	E665	D668	ILE	GLU	GLY	GLY	PHE	GLU	ASP	VAL	E678	Y679	T680	M681	S682	S683	L684	L685	N686	E687	G688	L689	I690	E691	Y692	I693	D694	A695	E696	F697	T698	P699	S700	I701	L702					
I703	A704	Q705	T706	D707	E708	D709	L710	E711	P712	A715	ASN	GLU	ASN	ASN	ASP	LEU	D722	V723	D724	K727	R728	I729	R730	V731	S732	H733	H734	H735	A736	T737	F738	T739	H740	C741	E742	I743	H744	P745	S746	M747	I748	N749	G750	V751	A752	F753	S754	I755	I756	F757	F758	P759	D760	H761	N762	V763	Q764	S764			
P765	R766	N767	Q768	Y769	Q770	S771	A772	M773	K775	Q776	R777	M778	G779	F780	F781	L782	T783	N784	Y785	N786	R787	R788	M789	D790	T791	M792	A793	N794	I795	L796	Y797	F798	Q800	K801	P802	L803	T806	R807	A808	M809	E810	L811	L812	K813	F814	R815	E816	L817	Q821	N822	A823	I824	V825	A826	L827						



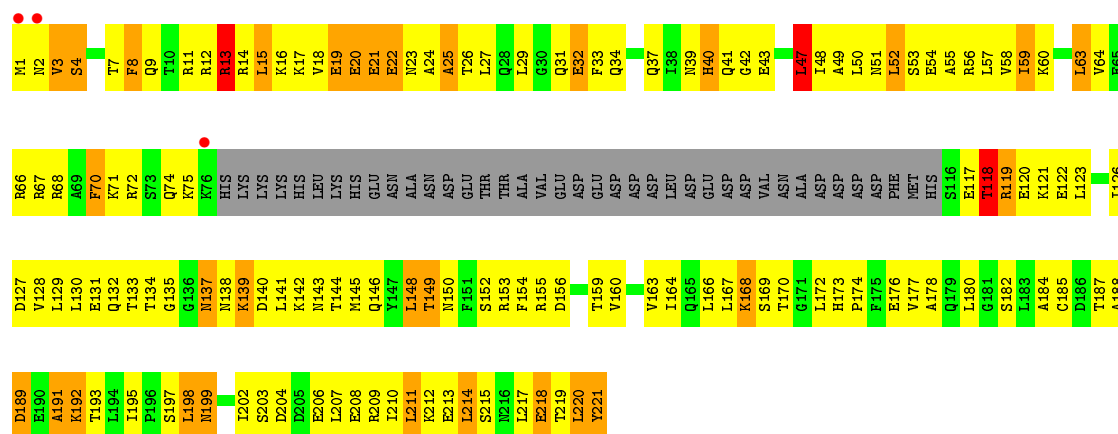
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 19% 52% 12% 17%

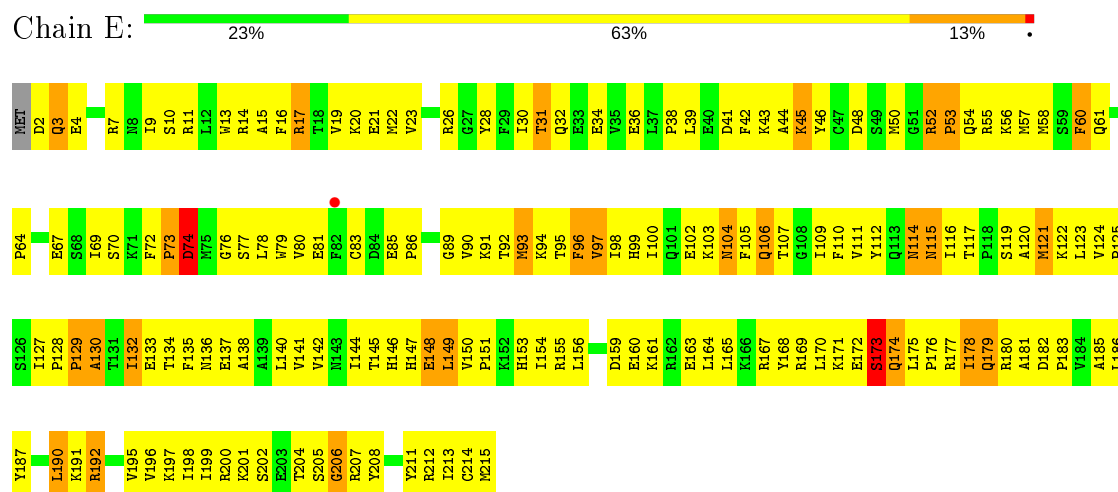


• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

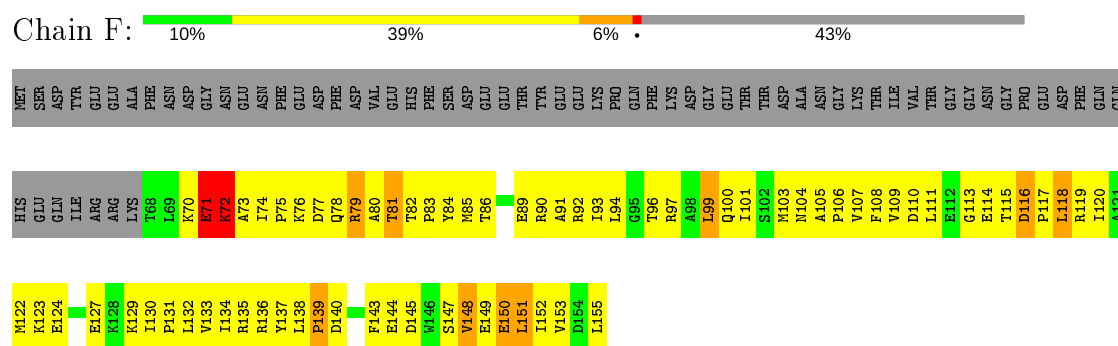
Chain D: 19% 48% 14% 18%



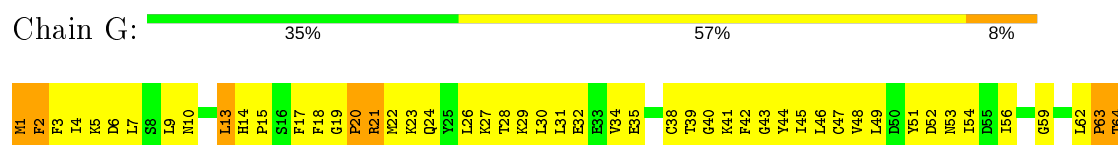
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

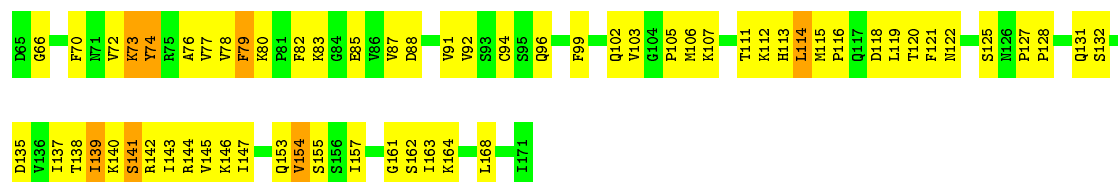


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

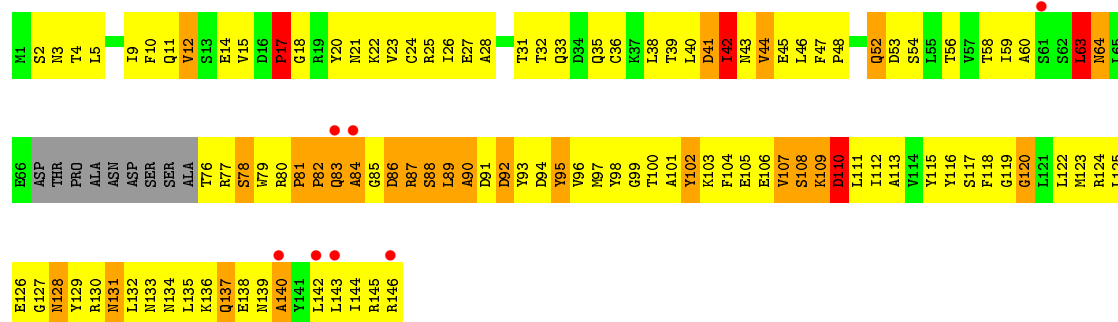
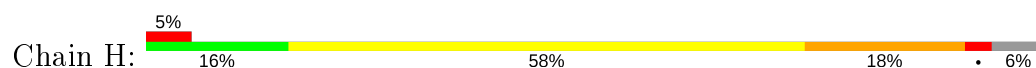


• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

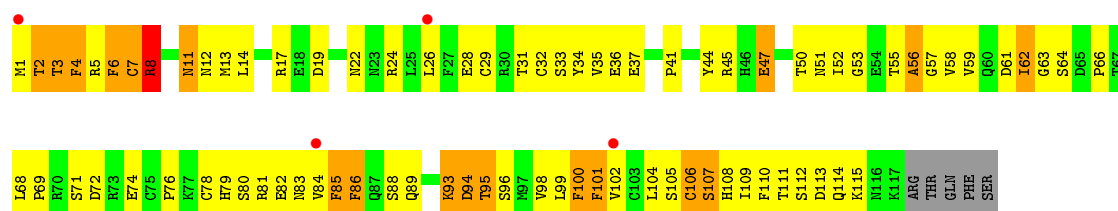




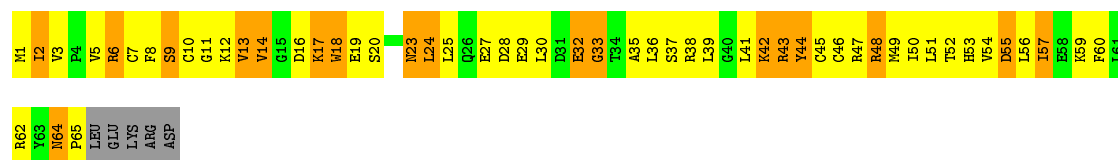
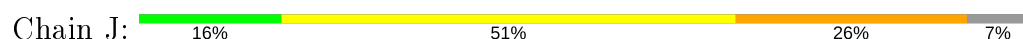
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



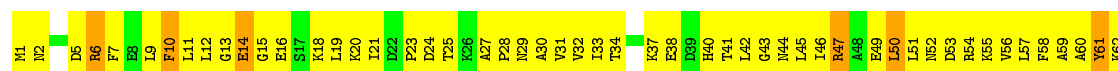
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11





- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 13: DNA (5'-D(*AP*G*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP*(8OG)P*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3')



- Molecule 14: DNA (5'-D(*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3')



- Molecule 15: RNA (5'-R(*UP*GP*CP*AP*UP*C*UP*UP*CP*CP*AP*GP*GP*CP*AP*U)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	221.17Å 394.15Å 282.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.90 49.81 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-3.90) 100.0 (49.81-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 3.88Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.228 , 0.266 0.214 , 0.253	Depositor DCC
R_{free} test set	4364 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	128.1	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 95.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.019 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32307	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 8OG, ZN, BRU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/11441	0.73	1/15473 (0.0%)
2	B	0.41	0/9116	0.69	1/12291 (0.0%)
3	C	0.42	0/2163	0.72	0/2930
4	D	0.39	0/1475	0.64	0/1976
5	E	0.39	0/1788	0.66	0/2406
6	F	0.46	0/724	0.82	0/977
7	G	0.44	0/1368	0.68	0/1844
8	H	0.38	0/1119	0.69	0/1514
9	I	0.36	0/970	0.66	0/1305
10	J	0.43	0/541	0.71	0/727
11	K	0.44	0/947	0.68	0/1279
12	L	0.45	0/372	0.75	0/495
13	T	0.61	0/405	0.84	0/618
14	N	0.67	0/251	0.93	0/386
15	P	0.54	0/230	0.82	0/356
All	All	0.42	0/32910	0.71	2/44577 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	882	THR	N-CA-C	5.61	126.14	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	567	LYS	C-N-CD	5.18	139.27	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	797	TYR	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11240	0	11313	1726	0
2	B	8942	0	8987	1312	0
3	C	2125	0	2090	327	0
4	D	1465	0	1489	212	0
5	E	1752	0	1776	229	0
6	F	712	0	738	127	0
7	G	1340	0	1357	167	0
8	H	1101	0	1075	211	0
9	I	952	0	913	140	0
10	J	532	0	542	113	0
11	K	929	0	939	132	0
12	L	370	0	394	89	0
13	T	407	0	225	43	0
14	N	224	0	126	11	0
15	P	207	0	109	9	0
16	A	1	0	0	0	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
All	All	32307	0	32073	4433	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 69.

All (4433) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.19	1.14
1:A:320:ARG:HB2	1:A:320:ARG:HH11	1.07	1.14
8:H:33:GLN:HE21	8:H:35:GLN:HB2	1.12	1.13
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.25	1.12
1:A:590:ARG:HH21	1:A:620:LYS:HB3	1.06	1.12
7:G:138:THR:HG22	7:G:139:ILE:H	1.05	1.12
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.32	1.12
2:B:638:PHE:HA	2:B:690:VAL:HG22	1.31	1.11
7:G:122:ASN:HD22	7:G:125:SER:HB3	1.11	1.10
3:C:66:ARG:HH12	10:J:2:ILE:HG21	0.96	1.10
2:B:806:THR:HG22	2:B:808:ALA:H	1.11	1.10
1:A:1244:ARG:HB3	1:A:1245:PRO:HA	1.21	1.09
1:A:567:LYS:HG3	8:H:95:TYR:HA	1.32	1.08
6:F:109:VAL:HG12	6:F:110:ASP:H	1.13	1.08
1:A:41:MET:HB2	1:A:49:LYS:HA	1.35	1.08
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.12	1.08
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.35	1.08
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.33	1.07
2:B:1095:LEU:HD12	2:B:1095:LEU:H	1.14	1.07
1:A:1006:ILE:HD11	5:E:163:GLU:HG3	1.38	1.06
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.30	1.05
2:B:642:ASP:HA	2:B:649:LYS:HA	1.36	1.05
1:A:1017:LEU:HB2	5:E:206:GLY:H	1.14	1.04
1:A:1424:VAL:HG13	1:A:1436:ILE:HD11	1.38	1.04
2:B:165:VAL:HG11	2:B:448:ILE:HD12	1.36	1.04
3:C:66:ARG:NH1	10:J:2:ILE:HG21	1.72	1.04
2:B:186:GLU:HG3	10:J:62:ARG:HH22	1.22	1.04
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.39	1.03
2:B:340:ALA:HB3	2:B:343:ILE:HG12	1.33	1.03
6:F:130:ILE:O	6:F:148:VAL:HG21	1.58	1.03
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.41	1.02
10:J:64:ASN:HB3	10:J:65:PRO:CD	1.88	1.02
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.42	1.02
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.41	1.01
1:A:108:MET:HB3	1:A:210:ILE:HD13	1.40	1.01
2:B:603:LEU:HB3	2:B:609:ILE:HD11	1.40	1.01
1:A:901:LEU:H	1:A:926:GLN:NE2	1.59	1.01
2:B:1099:VAL:HG13	2:B:1100:ASP:H	1.25	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:934:LYS:HG2	2:B:934:LYS:O	1.62	0.99
12:L:34:CYS:HB3	12:L:51:CYS:SG	2.03	0.99
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	1.97	0.99
1:A:53:LEU:HD23	1:A:54:ASN:N	1.77	0.99
3:C:43:THR:HG22	3:C:44:LEU:H	1.25	0.98
1:A:1409:LEU:HD13	2:B:1207:LEU:HD11	1.42	0.98
11:K:46:ILE:O	11:K:50:LEU:HB2	1.64	0.98
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.42	0.98
12:L:32:ALA:HB2	12:L:55:ILE:HG13	1.43	0.98
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.12	0.97
5:E:22:MET:HE3	5:E:26:ARG:HH11	1.27	0.97
2:B:882:THR:HG22	2:B:884:ARG:HB2	1.45	0.97
7:G:62:LEU:HB3	7:G:63:PRO:HD2	1.45	0.97
12:L:61:THR:HG22	12:L:63:ARG:H	1.26	0.97
4:D:134:THR:HG22	4:D:135:GLY:H	1.28	0.97
1:A:567:LYS:HE2	8:H:47:PHE:HB2	1.45	0.97
1:A:763:ALA:O	1:A:803:SER:HB3	1.65	0.97
2:B:746:SER:HB2	2:B:1046:PRO:HG2	1.46	0.97
2:B:1002:THR:CG2	2:B:1006:ILE:HG13	1.94	0.97
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.45	0.96
2:B:497:ARG:HH22	2:B:775:LYS:HE2	1.26	0.96
1:A:1445:ILE:HD12	1:A:1445:ILE:H	1.31	0.96
10:J:48:ARG:HE	10:J:49:MET:HE2	1.25	0.95
1:A:1254:ALA:O	1:A:1255:GLU:HB2	1.66	0.95
11:K:65:HIS:HD2	11:K:67:PHE:H	1.01	0.95
1:A:637:LYS:HB3	1:A:641:VAL:HG21	1.48	0.95
2:B:723:VAL:HG12	2:B:724:ASP:H	1.28	0.95
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.47	0.94
8:H:25:ARG:HA	8:H:41:ASP:HA	1.47	0.94
1:A:855:THR:HG21	1:A:857:ARG:HE	1.33	0.94
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.48	0.94
1:A:49:LYS:HZ1	1:A:61:ILE:H	1.11	0.94
11:K:65:HIS:CD2	11:K:67:PHE:H	1.85	0.94
3:C:244:VAL:O	3:C:248:ILE:HG13	1.68	0.94
2:B:611:PRO:HG2	2:B:685:LEU:HD21	1.50	0.94
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.33	0.93
1:A:666:ILE:HD12	1:A:667:GLY:H	1.31	0.93
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.32	0.93
4:D:47:LEU:HD13	4:D:48:ILE:H	1.32	0.93
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.29	0.93
2:B:559:SER:HA	2:B:563:MET:HB3	1.48	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.48	0.92
8:H:64:ASN:HB2	8:H:88:SER:HB2	1.50	0.92
1:A:754:SER:H	1:A:757:ASN:HD22	1.17	0.92
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.50	0.92
1:A:390:GLN:O	1:A:394:ASN:HB2	1.69	0.92
1:A:40:THR:HG22	1:A:41:MET:HG3	1.52	0.92
1:A:1369:ALA:O	1:A:1372:VAL:HG12	1.68	0.91
1:A:1160:SER:HA	1:A:1170:ILE:HD13	1.52	0.91
1:A:808:LEU:HD23	1:A:813:PHE:HA	1.52	0.91
2:B:944:THR:HG21	2:B:1122:ARG:NH2	1.85	0.91
1:A:1116:LEU:HB3	1:A:1308:THR:CG2	2.01	0.91
1:A:590:ARG:NH2	1:A:620:LYS:HB3	1.86	0.91
2:B:430:ARG:O	2:B:434:ARG:HD2	1.71	0.91
4:D:53:SER:H	4:D:148:LEU:CD2	1.84	0.90
5:E:22:MET:CE	5:E:26:ARG:HH11	1.83	0.90
12:L:26:THR:HG23	12:L:62:LYS:NZ	1.86	0.90
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.52	0.90
13:T:16:DT:H2''	13:T:17:DT:H5'	1.51	0.90
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.72	0.90
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.52	0.90
12:L:40:LEU:HD13	12:L:44:ASP:HB3	1.51	0.90
1:A:49:LYS:HZ1	1:A:61:ILE:N	1.70	0.90
1:A:1332:PHE:H	1:A:1332:PHE:HD2	1.13	0.90
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.07	0.90
11:K:31:VAL:HG12	11:K:32:VAL:H	1.36	0.90
2:B:654:ARG:H	2:B:657:HIS:HD2	1.17	0.89
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.53	0.89
10:J:64:ASN:HB3	10:J:65:PRO:HD2	1.51	0.89
1:A:567:LYS:CG	8:H:95:TYR:HA	2.02	0.89
2:B:1150:ARG:HG3	2:B:1150:ARG:HH11	1.37	0.89
7:G:138:THR:HG22	7:G:139:ILE:N	1.88	0.89
3:C:73:GLN:HE21	3:C:75:MET:H	1.21	0.89
4:D:168:LYS:HG3	4:D:177:VAL:HG11	1.53	0.89
1:A:567:LYS:HB2	8:H:96:VAL:H	1.38	0.89
1:A:665:GLY:O	1:A:667:GLY:N	2.06	0.89
1:A:1343:ALA:HB2	5:E:150:VAL:HG22	1.54	0.89
12:L:30:ILE:O	12:L:56:LEU:HA	1.72	0.89
1:A:1057:VAL:HG12	1:A:1058:VAL:H	1.38	0.88
2:B:515:HIS:H	2:B:518:HIS:HD2	1.18	0.88
3:C:61:GLU:HA	3:C:64:ALA:HB3	1.54	0.88
3:C:66:ARG:HH12	10:J:2:ILE:CG2	1.84	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:111:LEU:H	6:F:111:LEU:HD12	1.38	0.88
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.56	0.88
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.54	0.88
1:A:1244:ARG:HB3	1:A:1245:PRO:CA	2.03	0.88
2:B:364:ILE:O	2:B:365:THR:HB	1.72	0.88
2:B:882:THR:CG2	2:B:884:ARG:HB2	2.02	0.88
10:J:12:LYS:O	10:J:14:VAL:HG23	1.74	0.88
8:H:135:LEU:HD13	8:H:137:GLN:NE2	1.89	0.88
1:A:565:ILE:O	1:A:570:PRO:HA	1.74	0.88
1:A:308:ILE:HG22	1:A:309:ALA:H	1.39	0.88
1:A:320:ARG:HB2	1:A:320:ARG:NH1	1.89	0.87
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.56	0.87
4:D:11:ARG:HD2	4:D:31:GLN:HE22	1.38	0.87
1:A:946:VAL:HG13	5:E:201:LYS:HB3	1.54	0.87
9:I:111:THR:HG22	9:I:113:ASP:H	1.39	0.87
1:A:600:PRO:HG2	1:A:601:LYS:H	1.38	0.87
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.56	0.87
5:E:114:ASN:O	5:E:115:ASN:HB3	1.73	0.87
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.57	0.87
1:A:42:ASP:O	1:A:44:THR:N	2.08	0.87
1:A:962:ARG:HA	1:A:965:GLN:HB2	1.56	0.87
8:H:102:TYR:HD2	8:H:102:TYR:H	1.15	0.87
2:B:168:GLY:H	2:B:450:ALA:HB1	1.40	0.87
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.56	0.87
1:A:43:GLU:HB2	1:A:46:THR:HB	1.57	0.86
2:B:637:LEU:O	2:B:690:VAL:HG13	1.75	0.86
6:F:136:ARG:O	6:F:143:PHE:HB2	1.74	0.86
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	1.75	0.86
5:E:117:THR:HG22	5:E:119:SER:H	1.37	0.86
2:B:46:GLN:HG3	2:B:47:GLN:H	1.39	0.86
11:K:12:LEU:HD12	11:K:12:LEU:H	1.40	0.86
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.39	0.86
3:C:148:ARG:H	3:C:151:GLN:HG3	1.40	0.86
3:C:38:ILE:HA	3:C:173:ALA:HB2	1.58	0.86
1:A:666:ILE:H	2:B:1026:LEU:HD13	1.39	0.86
4:D:71:LYS:HG2	4:D:74:GLN:NE2	1.89	0.86
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.55	0.86
1:A:466:SER:HB3	2:B:1103:ILE:HG12	1.57	0.86
2:B:1165:ILE:HD11	4:D:17:LYS:HD3	1.57	0.86
2:B:126:SER:OG	2:B:172:ILE:HD11	1.75	0.85
2:B:842:ASN:HD22	2:B:845:SER:HB3	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:13:DT:H2''	13:T:14:DA:OP2	1.74	0.85
6:F:109:VAL:HG12	6:F:110:ASP:N	1.89	0.85
2:B:880:THR:HB	2:B:934:LYS:HD3	1.57	0.85
7:G:122:ASN:ND2	7:G:125:SER:HB3	1.91	0.85
1:A:1261:LYS:O	1:A:1264:GLU:HB3	1.76	0.85
1:A:537:ARG:HD2	8:H:20:TYR:HE1	1.41	0.85
14:N:3:DT:H1'	14:N:4:DA:C8	2.12	0.85
2:B:776:GLN:OE1	15:P:9:C:H4'	1.76	0.85
1:A:470:LEU:HD13	1:A:487:MET:HE1	1.59	0.85
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.57	0.85
1:A:180:LYS:NZ	1:A:294:SER:HB3	1.92	0.85
12:L:61:THR:HG21	12:L:63:ARG:HE	1.42	0.85
1:A:30:ILE:HG23	2:B:1170:THR:HG23	1.59	0.85
12:L:32:ALA:CB	12:L:55:ILE:HG13	2.07	0.85
1:A:196:GLU:HB2	1:A:197:PRO:HD2	1.58	0.85
2:B:1181:GLU:O	2:B:1182:CYS:HB3	1.74	0.85
1:A:2:VAL:HG11	2:B:1157:ALA:HB1	1.59	0.84
1:A:70:CYS:O	1:A:72:GLU:HG2	1.77	0.84
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.59	0.84
6:F:103:MET:CE	7:G:66:GLY:H	1.88	0.84
1:A:98:LYS:O	1:A:102:VAL:HG23	1.77	0.84
6:F:86:THR:OG1	6:F:89:GLU:HG3	1.77	0.84
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.11	0.84
8:H:128:ASN:H	8:H:130:ARG:NH1	1.75	0.84
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.59	0.84
1:A:372:LYS:HA	1:A:435:HIS:ND1	1.91	0.84
3:C:6:PRO:HB2	11:K:101:LEU:HD12	1.57	0.84
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.57	0.84
12:L:55:ILE:HD13	12:L:55:ILE:H	1.41	0.84
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	1.78	0.84
4:D:118:THR:HG21	4:D:121:LYS:HD2	1.57	0.84
13:T:15:DC:H2''	13:T:16:DT:H71	1.57	0.84
2:B:882:THR:HG21	2:B:935:ARG:HA	1.59	0.84
3:C:43:THR:HG22	3:C:44:LEU:N	1.92	0.84
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.57	0.84
1:A:35:ILE:HG22	1:A:84:ILE:HD12	1.58	0.84
1:A:746:MET:CE	2:B:1018:PRO:HG2	2.07	0.84
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.59	0.84
8:H:15:VAL:HG13	8:H:26:ILE:HG12	1.60	0.84
1:A:1047:SER:O	1:A:1050:GLU:HB3	1.77	0.84
1:A:225:ASN:ND2	1:A:228:PHE:H	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:664:THR:HG1	2:B:678:GLU:N	1.75	0.84
1:A:442:VAL:HG12	1:A:490:HIS:O	1.78	0.83
5:E:180:ARG:NH2	5:E:192:ARG:HB2	1.94	0.83
12:L:26:THR:HG23	12:L:62:LYS:HZ3	1.44	0.83
2:B:824:ILE:HG22	2:B:1087:PHE:HE2	1.41	0.83
1:A:470:LEU:HD23	1:A:470:LEU:H	1.44	0.83
2:B:515:HIS:HD2	2:B:517:THR:H	1.22	0.83
2:B:1159:ARG:NH1	2:B:1159:ARG:HB3	1.93	0.83
4:D:139:LYS:HE2	4:D:143:ASN:HD21	1.42	0.83
10:J:48:ARG:HD2	10:J:49:MET:N	1.92	0.83
1:A:188:ASP:HB3	1:A:191:THR:HB	1.60	0.83
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.42	0.83
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.78	0.83
1:A:384:ASN:OD1	1:A:388:LEU:HD12	1.78	0.82
2:B:469:GLN:HG3	2:B:470:LYS:H	1.45	0.82
5:E:197:LYS:HE2	5:E:199:ILE:HD11	1.60	0.82
2:B:515:HIS:H	2:B:518:HIS:CD2	1.96	0.82
13:T:24:DG:H2'	13:T:25:DG:C8	2.14	0.82
1:A:84:ILE:HD11	1:A:270:LEU:HD13	1.62	0.82
3:C:32:SER:O	3:C:36:VAL:HG23	1.80	0.82
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.61	0.82
1:A:49:LYS:NZ	1:A:61:ILE:H	1.78	0.81
1:A:857:ARG:HD3	1:A:861:GLY:O	1.79	0.81
4:D:34:GLN:O	4:D:47:LEU:HD23	1.79	0.81
8:H:26:ILE:HG22	8:H:27:GLU:H	1.45	0.81
10:J:8:PHE:H	10:J:49:MET:HE1	1.45	0.81
5:E:78:LEU:HA	5:E:107:THR:HB	1.63	0.81
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.44	0.81
1:A:567:LYS:HB3	1:A:568:PRO:HD3	1.62	0.81
2:B:706:GLN:HE21	2:B:730:ARG:HH11	1.29	0.81
4:D:18:VAL:O	4:D:19:GLU:HB2	1.79	0.81
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.11	0.81
10:J:35:ALA:O	10:J:39:LEU:HD12	1.80	0.81
1:A:255:SER:OG	2:B:918:ILE:CG2	2.27	0.81
2:B:193:LYS:NZ	12:L:32:ALA:HB1	1.96	0.81
13:T:9:DC:H2''	13:T:10:DA:C8	2.15	0.81
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.61	0.81
3:C:20:PHE:HE1	3:C:22:LEU:HB2	1.45	0.81
4:D:8:PHE:HZ	4:D:37:GLN:HB2	1.46	0.81
8:H:100:THR:OG1	8:H:138:GLU:HG3	1.81	0.81
2:B:1099:VAL:HG13	2:B:1100:ASP:N	1.96	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.61	0.81
2:B:288:ALA:HA	2:B:331:LEU:HD12	1.62	0.81
3:C:142:VAL:H	10:J:16:ASP:HB3	1.46	0.81
2:B:1165:ILE:CD1	4:D:17:LYS:HD3	2.10	0.81
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.11	0.81
2:B:378:LEU:O	2:B:382:ILE:HG13	1.81	0.81
1:A:320:ARG:CB	1:A:320:ARG:HH11	1.91	0.81
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.62	0.81
4:D:155:ARG:HD3	4:D:221:TYR:CZ	2.16	0.81
5:E:17:ARG:HB2	5:E:17:ARG:HH11	1.43	0.81
12:L:55:ILE:O	12:L:56:LEU:HB2	1.81	0.81
2:B:503:GLY:HA3	2:B:507:LYS:HE2	1.61	0.80
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.61	0.80
4:D:8:PHE:HD2	7:G:6:ASP:HB2	1.45	0.80
1:A:535:THR:HG21	1:A:616:VAL:HA	1.63	0.80
3:C:66:ARG:HH21	10:J:5:VAL:HG23	1.46	0.80
1:A:1435:PRO:HA	1:A:1439:GLY:O	1.82	0.80
1:A:903:ASN:HD22	1:A:904:THR:H	1.26	0.80
2:B:1115:THR:HG22	2:B:1117:GLN:HG3	1.63	0.80
5:E:178:ILE:HB	5:E:212:ARG:HD2	1.63	0.80
1:A:741:ASN:ND2	1:A:744:LYS:H	1.80	0.80
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.46	0.80
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.46	0.80
5:E:17:ARG:NH1	5:E:17:ARG:HB2	1.97	0.80
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.63	0.80
1:A:1187:GLN:O	1:A:1244:ARG:HG3	1.81	0.80
1:A:1187:GLN:HG3	1:A:1188:GLN:HG3	1.64	0.80
1:A:855:THR:CG2	1:A:857:ARG:HE	1.94	0.80
4:D:71:LYS:HG2	4:D:74:GLN:HE21	1.45	0.80
6:F:103:MET:HE2	7:G:66:GLY:H	1.43	0.80
11:K:21:ILE:HG22	11:K:31:VAL:HG11	1.64	0.80
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.22	0.80
13:T:10:DA:H2"	13:T:11:DA:C8	2.16	0.80
4:D:40:HIS:CD2	7:G:73:LYS:HG2	2.17	0.80
1:A:524:VAL:HG12	1:A:525:GLN:N	1.97	0.79
5:E:156:LEU:HD12	5:E:195:VAL:HB	1.62	0.79
1:A:41:MET:CB	1:A:49:LYS:HA	2.11	0.79
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.64	0.79
2:B:193:LYS:HD3	2:B:787:VAL:HG11	1.65	0.79
2:B:746:SER:CB	2:B:1046:PRO:HG2	2.13	0.79
2:B:186:GLU:HG3	10:J:62:ARG:NH2	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:ILE:O	1:A:580:VAL:HG23	1.83	0.79
5:E:19:VAL:O	5:E:23:VAL:HG23	1.82	0.79
1:A:1447:GLU:OE2	7:G:23:LYS:HB2	1.83	0.79
1:A:323:LYS:H	1:A:323:LYS:HD2	1.47	0.79
1:A:825:ILE:HD11	2:B:512:ARG:HD3	1.65	0.79
3:C:8:VAL:O	3:C:9:LYS:HG3	1.81	0.79
4:D:180:LEU:HD23	4:D:195:ILE:HD12	1.63	0.79
6:F:82:THR:HG22	6:F:84:TYR:H	1.47	0.79
1:A:117:GLU:H	1:A:117:GLU:CD	1.86	0.79
1:A:809:THR:H	1:A:812:GLU:HB2	1.46	0.79
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.65	0.79
4:D:71:LYS:HA	4:D:74:GLN:HG3	1.65	0.79
1:A:829:VAL:HG11	2:B:508:LEU:HD22	1.63	0.79
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	1.97	0.79
5:E:31:THR:HG23	5:E:34:GLU:HB2	1.65	0.79
8:H:100:THR:HG23	8:H:138:GLU:HA	1.65	0.79
1:A:472:LEU:O	1:A:475:THR:HB	1.82	0.79
2:B:1183:LYS:O	2:B:1185:CYS:N	2.15	0.78
2:B:745:PRO:O	2:B:748:ILE:HG12	1.84	0.78
12:L:30:ILE:O	12:L:56:LEU:HD23	1.83	0.78
2:B:821:GLN:HE22	2:B:851:PHE:H	1.30	0.78
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.48	0.78
6:F:99:LEU:O	6:F:103:MET:HG2	1.83	0.78
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.65	0.78
2:B:516:ASN:N	2:B:516:ASN:HD22	1.77	0.78
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.64	0.78
10:J:44:TYR:HD2	10:J:44:TYR:H	1.29	0.78
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.63	0.78
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.65	0.78
1:A:590:ARG:HB3	1:A:605:MET:H	1.48	0.78
2:B:830:TYR:HE2	2:B:1000:PRO:HD3	1.48	0.78
1:A:1057:VAL:HG12	1:A:1058:VAL:N	1.98	0.78
2:B:277:LYS:HG3	2:B:338:GLY:HA2	1.66	0.78
1:A:1030:ARG:HG3	1:A:1034:GLU:OE2	1.83	0.78
1:A:849:MET:HE1	1:A:1061:GLY:HA2	1.63	0.78
4:D:213:GLU:O	4:D:217:LEU:HG	1.84	0.78
2:B:217:ARG:NE	2:B:405:ARG:HB2	1.98	0.78
2:B:345:LYS:O	2:B:347:LYS:HG2	1.84	0.78
1:A:560:ILE:HD11	8:H:79:TRP:H	1.47	0.78
1:A:372:LYS:HA	1:A:435:HIS:HD1	1.48	0.78
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:21:DC:H2''	13:T:22:DC:H5'	1.64	0.78
1:A:1130:GLN:HG3	1:A:1134:ILE:HD11	1.65	0.77
2:B:345:LYS:O	2:B:347:LYS:N	2.17	0.77
7:G:13:LEU:HD23	7:G:14:HIS:H	1.49	0.77
4:D:8:PHE:CD2	7:G:6:ASP:HB2	2.18	0.77
1:A:266:LEU:HD21	1:A:303:TYR:CE1	2.20	0.77
7:G:128:PRO:O	7:G:138:THR:HG23	1.83	0.77
2:B:826:ALA:HB2	2:B:1008:PRO:HB3	1.67	0.77
2:B:46:GLN:HB2	2:B:408:LEU:HD21	1.64	0.77
1:A:1008:GLN:O	1:A:1011:GLN:HB3	1.85	0.77
1:A:1227:ILE:HG22	1:A:1228:TRP:N	1.99	0.77
2:B:244:LEU:HD11	2:B:366:GLN:HE22	1.49	0.77
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.10	0.77
2:B:852:ARG:HH22	12:L:70:ARG:C	1.88	0.77
2:B:879:ARG:NH1	2:B:883:LEU:HD23	1.98	0.77
4:D:8:PHE:CZ	4:D:37:GLN:HB2	2.19	0.77
1:A:896:ARG:NH2	1:A:1030:ARG:HE	1.82	0.77
2:B:212:LEU:HD23	2:B:480:SER:HB2	1.65	0.77
13:T:15:DC:C2'	13:T:16:DT:H71	2.14	0.77
1:A:305:ASP:OD2	1:A:326:ARG:HD2	1.84	0.77
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.32	0.77
7:G:127:PRO:HG2	7:G:138:THR:HG21	1.67	0.77
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.65	0.77
1:A:1027:ALA:O	1:A:1031:VAL:HG23	1.84	0.77
2:B:430:ARG:O	2:B:434:ARG:CD	2.32	0.77
4:D:173:HIS:HD2	4:D:174:PRO:HD2	1.48	0.77
8:H:40:LEU:HB2	8:H:123:MET:HE3	1.65	0.77
1:A:1081:LEU:HD11	1:A:1098:VAL:H	1.48	0.77
1:A:1268:LEU:O	1:A:1269:GLU:HG3	1.85	0.77
2:B:879:ARG:O	2:B:934:LYS:HE2	1.85	0.77
1:A:382:PRO:HD3	1:A:428:TYR:HD2	1.49	0.77
2:B:120:ARG:NE	2:B:955:THR:HG21	1.99	0.77
3:C:238:ILE:HD13	3:C:246:ARG:HH11	1.50	0.77
7:G:115:MET:HB2	7:G:116:PRO:HD2	1.66	0.77
11:K:50:LEU:HD11	11:K:75:ILE:HD13	1.67	0.77
1:A:55:ASP:C	1:A:57:ARG:H	1.84	0.76
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.11	0.76
2:B:497:ARG:NH2	2:B:775:LYS:HE2	2.00	0.76
5:E:23:VAL:HG13	5:E:78:LEU:HD13	1.66	0.76
8:H:91:ASP:O	8:H:93:TYR:N	2.16	0.76
2:B:794:ASN:C	2:B:795:ILE:HD12	2.06	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.50	0.76
1:A:1116:LEU:HB3	1:A:1308:THR:HG22	1.66	0.76
1:A:995:GLU:OE1	1:A:995:GLU:HA	1.84	0.76
2:B:810:GLU:HB2	2:B:815:ARG:HH22	1.48	0.76
2:B:661:LEU:HD23	2:B:679:TYR:O	1.85	0.76
4:D:134:THR:HG22	4:D:135:GLY:N	1.99	0.76
2:B:579:ARG:HA	2:B:589:VAL:HG22	1.68	0.76
2:B:549:THR:HB	2:B:628:THR:OG1	1.85	0.76
4:D:57:LEU:HD11	4:D:160:VAL:HG21	1.66	0.76
5:E:180:ARG:HH21	5:E:192:ARG:CB	1.97	0.76
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.67	0.76
4:D:24:ALA:C	4:D:26:THR:H	1.88	0.76
1:A:230:ARG:H	1:A:233:TRP:HE3	1.34	0.76
1:A:903:ASN:HD22	1:A:904:THR:N	1.84	0.76
2:B:430:ARG:O	2:B:434:ARG:HG3	1.86	0.76
9:I:74:GLU:HA	9:I:80:SER:O	1.86	0.76
1:A:7:SER:HB3	2:B:1175:LEU:HD22	1.68	0.76
9:I:105:SER:O	9:I:106:CYS:HB3	1.85	0.76
1:A:534:LEU:O	1:A:574:GLY:HA3	1.86	0.76
7:G:153:GLN:HG2	7:G:154:VAL:HG23	1.68	0.76
8:H:130:ARG:HB3	8:H:134:ASN:HB2	1.66	0.76
2:B:1150:ARG:CG	2:B:1150:ARG:HH11	1.99	0.76
1:A:1325:THR:O	5:E:148:GLU:HB2	1.86	0.76
1:A:672:ASP:HB3	1:A:675:THR:HB	1.68	0.75
2:B:123:THR:OG1	2:B:458:LYS:HE2	1.86	0.75
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.00	0.75
3:C:101:LEU:O	3:C:102:GLN:HG3	1.85	0.75
1:A:1130:GLN:O	1:A:1134:ILE:HG13	1.85	0.75
1:A:317:LYS:HA	2:B:471:LYS:HE2	1.68	0.75
1:A:910:PRO:HB3	1:A:917:SER:H	1.51	0.75
7:G:138:THR:CG2	7:G:139:ILE:H	1.89	0.75
8:H:26:ILE:O	8:H:27:GLU:HG3	1.86	0.75
10:J:64:ASN:HD22	10:J:65:PRO:HD3	1.48	0.75
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	1.99	0.75
2:B:1095:LEU:HD12	2:B:1095:LEU:N	1.98	0.75
2:B:806:THR:HG22	2:B:808:ALA:N	1.95	0.75
1:A:107:CYS:N	1:A:114:LEU:HD21	2.01	0.75
2:B:168:GLY:HA2	2:B:454:THR:OG1	1.87	0.75
2:B:866:TYR:O	2:B:868:MET:N	2.19	0.75
4:D:144:THR:O	4:D:148:LEU:HB2	1.86	0.75
8:H:84:ALA:HB2	8:H:87:ARG:HD2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:SER:HA	1:A:233:TRP:NE1	2.02	0.75
1:A:695:LYS:HA	1:A:698:GLN:HB2	1.67	0.75
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.69	0.75
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.22	0.75
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.68	0.75
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.68	0.75
1:A:1148:ILE:HD11	1:A:1198:ASP:HA	1.69	0.75
1:A:898:ARG:HD2	1:A:899:VAL:H	1.52	0.75
2:B:577:ALA:CB	2:B:589:VAL:HG11	2.10	0.75
2:B:789:MET:HE2	2:B:965:LYS:HB3	1.68	0.75
1:A:135:PHE:HD1	1:A:222:LEU:HD22	1.51	0.75
2:B:101:MET:HB2	2:B:169:ARG:HH22	1.52	0.75
2:B:293:PRO:HG2	2:B:296:GLU:HB3	1.68	0.75
1:A:380:VAL:HG12	1:A:428:TYR:HA	1.69	0.75
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.67	0.75
10:J:23:ASN:C	10:J:25:LEU:H	1.90	0.75
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	2.01	0.74
1:A:302:THR:HA	1:A:305:ASP:O	1.87	0.74
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.87	0.74
9:I:6:PHE:HB3	9:I:12:ASN:O	1.86	0.74
3:C:7:GLN:HG2	11:K:104:ASN:ND2	2.01	0.74
1:A:12:ARG:HB2	2:B:1218:THR:HG22	1.68	0.74
1:A:148:CYS:O	1:A:168:GLY:HA2	1.86	0.74
1:A:697:ALA:HB2	1:A:702:LEU:HD12	1.69	0.74
9:I:111:THR:HG22	9:I:113:ASP:N	2.01	0.74
13:T:18:DA:H1'	13:T:19:8OG:H5'	1.69	0.74
2:B:326:ASP:OD2	2:B:328:GLU:HB3	1.86	0.74
2:B:497:ARG:HH22	2:B:775:LYS:CE	1.99	0.74
2:B:636:PRO:O	2:B:743:ILE:HD11	1.88	0.74
4:D:148:LEU:O	4:D:152:SER:HB3	1.87	0.74
11:K:107:THR:O	11:K:111:LEU:HG	1.87	0.74
1:A:438:ASP:O	1:A:439:ASN:HB2	1.85	0.74
4:D:159:THR:O	4:D:163:VAL:HG23	1.87	0.74
5:E:97:VAL:HG13	5:E:127:ILE:HD13	1.69	0.74
1:A:1193:LEU:HB2	1:A:1260:LEU:HD11	1.69	0.74
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.17	0.74
3:C:174:ALA:O	10:J:10:CYS:HB2	1.88	0.74
2:B:1002:THR:HG23	2:B:1006:ILE:HG13	1.68	0.74
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	1.87	0.74
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.68	0.74
1:A:403:LYS:O	1:A:415:LEU:HB2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:PHE:HA	1:A:595:THR:HG21	1.70	0.74
2:B:807:ARG:HG2	2:B:1045:SER:OG	1.86	0.74
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.70	0.74
10:J:1:MET:H1	10:J:57:ILE:H	1.33	0.74
14:N:3:DT:H4'	14:N:4:DA:H5'	1.70	0.74
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.70	0.74
3:C:259:LEU:HD21	11:K:91:CYS:HB3	1.68	0.74
3:C:76:ASP:O	3:C:78:GLU:N	2.21	0.74
1:A:135:PHE:CD1	1:A:222:LEU:HD22	2.22	0.74
1:A:808:LEU:HG	1:A:812:GLU:HB3	1.70	0.74
1:A:933:TYR:O	1:A:937:VAL:HG23	1.88	0.74
6:F:75:PRO:HG2	6:F:77:ASP:O	1.87	0.74
1:A:1009:ASN:HA	1:A:1012:ARG:NH1	2.02	0.73
2:B:351:TYR:O	2:B:355:ILE:HG13	1.89	0.73
1:A:825:ILE:HD11	2:B:512:ARG:HB3	1.70	0.73
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.68	0.73
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.23	0.73
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.23	0.73
8:H:99:GLY:HA3	8:H:118:PHE:HA	1.69	0.73
1:A:567:LYS:HG3	8:H:94:ASP:O	1.88	0.73
2:B:60:GLN:O	2:B:63:ILE:HG22	1.88	0.73
3:C:115:SER:HB3	3:C:142:VAL:HB	1.69	0.73
8:H:130:ARG:N	8:H:130:ARG:HD2	2.03	0.73
1:A:215:SER:HB3	1:A:218:ASP:OD2	1.87	0.73
1:A:71:GLN:HG3	1:A:72:GLU:H	1.54	0.73
2:B:526:GLU:HG2	2:B:538:ASN:HD22	1.54	0.73
3:C:101:LEU:CD1	3:C:118:LEU:HD23	2.15	0.73
3:C:148:ARG:N	3:C:151:GLN:HG3	2.02	0.73
11:K:82:ASP:OD1	11:K:84:LYS:HG3	1.88	0.73
8:H:81:PRO:HG2	8:H:82:PRO:HD2	1.69	0.73
11:K:65:HIS:HD2	11:K:67:PHE:N	1.84	0.73
1:A:825:ILE:CD1	2:B:512:ARG:HB3	2.18	0.73
1:A:849:MET:HB2	1:A:1062:GLU:O	1.89	0.73
1:A:87:ALA:HB1	1:A:276:LEU:HD23	1.70	0.73
1:A:896:ARG:HH21	1:A:1030:ARG:NE	1.87	0.73
1:A:919:ILE:HG23	1:A:925:LEU:HD12	1.70	0.73
7:G:102:GLN:HG3	7:G:106:MET:O	1.88	0.73
13:T:7:DC:H2''	13:T:8:DT:C5	2.24	0.73
1:A:709:THR:HG22	1:A:711:ARG:H	1.54	0.73
2:B:220:GLY:O	2:B:222:ILE:HG13	1.89	0.73
4:D:60:LYS:O	4:D:64:VAL:HG23	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:129:TYR:HA	8:H:131:ASN:ND2	2.04	0.73
2:B:216:GLU:HB3	2:B:500:THR:HG23	1.70	0.73
2:B:613:VAL:HG22	2:B:628:THR:HA	1.70	0.73
3:C:98:VAL:C	3:C:99:LEU:HD23	2.09	0.73
1:A:701:LEU:HD21	9:I:114:GLN:HB2	1.71	0.73
2:B:230:ALA:N	2:B:231:PRO:HD2	2.04	0.73
4:D:137:ASN:ND2	4:D:137:ASN:H	1.87	0.73
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.71	0.73
1:A:1198:ASP:HB3	1:A:1201:ALA:HB3	1.71	0.72
2:B:906:SER:O	2:B:941:LEU:HD23	1.89	0.72
5:E:92:THR:O	5:E:95:THR:HB	1.89	0.72
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.70	0.72
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.71	0.72
1:A:963:ILE:HD13	1:A:1049:ILE:HG12	1.71	0.72
2:B:335:GLY:HA3	2:B:348:ARG:HB2	1.71	0.72
2:B:95:ILE:HB	2:B:130:VAL:HG22	1.71	0.72
3:C:62:PHE:O	3:C:66:ARG:HG3	1.89	0.72
11:K:21:ILE:HG23	11:K:33:ILE:HG12	1.71	0.72
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.71	0.72
1:A:167:CYS:HB2	1:A:169:ASN:ND2	2.03	0.72
1:A:847:ASP:OD2	1:A:858:ASN:HB2	1.89	0.72
7:G:88:ASP:HB3	7:G:144:ARG:HA	1.70	0.72
1:A:37:PHE:H	1:A:37:PHE:HD1	1.38	0.72
1:A:855:THR:HG21	1:A:857:ARG:NE	2.04	0.72
5:E:61:GLN:HG3	5:E:78:LEU:O	1.90	0.72
1:A:1002:GLY:HA3	1:A:1007:ILE:CG2	2.19	0.72
1:A:774:ARG:NH1	1:A:797:LYS:HG3	2.04	0.72
4:D:139:LYS:HE2	4:D:143:ASN:ND2	2.03	0.72
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.72	0.72
1:A:1308:THR:HG23	1:A:1309:ASP:N	2.03	0.72
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.70	0.72
1:A:567:LYS:HD2	8:H:95:TYR:CD2	2.25	0.72
2:B:112:LEU:HD12	2:B:113:TYR:H	1.54	0.72
6:F:109:VAL:CG1	6:F:110:ASP:H	1.97	0.72
1:A:100:LYS:HE2	1:A:104:GLU:OE2	1.89	0.72
1:A:1332:PHE:N	1:A:1332:PHE:CD2	2.55	0.72
1:A:646:PHE:O	1:A:650:GLN:HB2	1.90	0.72
1:A:332:LYS:H	1:A:337:ARG:HB3	1.55	0.72
1:A:524:VAL:HG12	1:A:525:GLN:H	1.54	0.72
1:A:71:GLN:HG3	1:A:72:GLU:N	2.04	0.72
2:B:23:ALA:H	2:B:654:ARG:HB3	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.70	0.72
1:A:1045:VAL:O	1:A:1049:ILE:HG13	1.90	0.72
1:A:53:LEU:HD23	1:A:54:ASN:H	1.53	0.72
1:A:751:SER:O	1:A:752:LYS:HG2	1.89	0.72
1:A:885:THR:O	1:A:940:ARG:HD2	1.88	0.72
2:B:118:ARG:HG2	2:B:204:ILE:HD13	1.72	0.72
7:G:40:GLY:HA2	7:G:157:ILE:HD11	1.72	0.72
8:H:36:CYS:HA	8:H:126:GLU:O	1.89	0.72
1:A:71:GLN:CG	1:A:72:GLU:H	2.00	0.72
2:B:435:THR:HG22	2:B:435:THR:O	1.89	0.72
2:B:801:LYS:O	10:J:52:THR:HG23	1.89	0.72
5:E:52:ARG:HB3	5:E:53:PRO:HD2	1.71	0.72
8:H:38:LEU:HD12	8:H:124:ARG:O	1.90	0.72
12:L:32:ALA:HB3	12:L:33:GLU:OE2	1.89	0.72
1:A:1237:ILE:HG22	1:A:1238:ILE:N	2.05	0.71
1:A:1315:GLU:C	1:A:1317:MET:H	1.92	0.71
3:C:128:ASN:O	3:C:129:ILE:HG13	1.90	0.71
8:H:89:LEU:C	8:H:91:ASP:H	1.91	0.71
1:A:265:LYS:HE2	1:A:302:THR:HG23	1.72	0.71
1:A:567:LYS:HG3	8:H:95:TYR:CA	2.17	0.71
2:B:1085:ILE:HD12	2:B:1085:ILE:N	2.05	0.71
1:A:34:LYS:CB	1:A:36:ARG:HH21	2.03	0.71
1:A:32:VAL:HG21	1:A:68:GLN:NE2	2.05	0.71
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.20	0.71
2:B:1183:LYS:HA	2:B:1186:ASP:HA	1.70	0.71
6:F:72:LYS:HA	6:F:72:LYS:HE3	1.72	0.71
1:A:55:ASP:CG	1:A:55:ASP:O	2.29	0.71
1:A:629:LEU:O	1:A:633:VAL:HG23	1.89	0.71
2:B:277:LYS:O	2:B:278:GLN:HB2	1.88	0.71
2:B:999:MET:HA	2:B:999:MET:CE	2.20	0.71
7:G:62:LEU:HB3	7:G:63:PRO:CD	2.18	0.71
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.55	0.71
2:B:954:VAL:HG13	2:B:964:VAL:HG22	1.72	0.71
3:C:20:PHE:CE1	3:C:22:LEU:HB2	2.25	0.71
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.25	0.71
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.71	0.71
3:C:268:ASP:O	3:C:269:LYS:HB2	1.90	0.71
7:G:9:LEU:HD12	7:G:10:ASN:N	2.04	0.71
1:A:822:GLU:O	1:A:825:ILE:HG22	1.90	0.71
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.73	0.71
2:B:179:CYS:SG	2:B:181:LEU:HD12	2.30	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:124:VAL:N	5:E:125:PRO:HD2	2.04	0.71
6:F:80:ALA:HB3	6:F:144:GLU:OE2	1.91	0.71
1:A:590:ARG:HH21	1:A:620:LYS:CB	1.96	0.71
8:H:128:ASN:H	8:H:130:ARG:HH11	1.39	0.71
12:L:40:LEU:HD22	12:L:44:ASP:CG	2.11	0.71
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.55	0.71
1:A:901:LEU:H	1:A:926:GLN:HE21	1.37	0.71
2:B:313:MET:O	2:B:316:PRO:HD2	1.91	0.71
2:B:603:LEU:HD12	2:B:609:ILE:HG12	1.73	0.71
4:D:208:GLU:HG3	4:D:212:LYS:HE3	1.73	0.71
11:K:68:PHE:HB3	11:K:70:ARG:HH11	1.55	0.71
2:B:359:GLU:O	2:B:362:PRO:HD3	1.91	0.71
6:F:135:ARG:HG2	6:F:137:TYR:CE1	2.26	0.71
7:G:143:ILE:HG22	7:G:144:ARG:N	2.05	0.71
1:A:92:HIS:HB2	1:A:236:LEU:HD21	1.71	0.70
1:A:853:ASP:O	1:A:854:ASN:HB2	1.91	0.70
1:A:868:TYR:OH	1:A:1366:ARG:HD3	1.90	0.70
3:C:193:TYR:HD2	3:C:197:SER:HB3	1.54	0.70
3:C:256:ALA:HA	3:C:259:LEU:HD23	1.72	0.70
1:A:332:LYS:CA	1:A:337:ARG:HD2	2.21	0.70
1:A:888:GLY:O	1:A:940:ARG:NH2	2.24	0.70
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.56	0.70
2:B:1215:ARG:NH1	4:D:15:LEU:HD21	2.05	0.70
6:F:97:ARG:O	6:F:101:ILE:HG13	1.92	0.70
2:B:900:ALA:HB3	12:L:61:THR:OG1	1.91	0.70
1:A:10:PRO:HB3	4:D:3:VAL:HA	1.73	0.70
1:A:896:ARG:HH21	1:A:1030:ARG:HE	1.35	0.70
1:A:7:SER:CB	2:B:1175:LEU:HD22	2.20	0.70
1:A:315:LEU:HD13	2:B:471:LYS:HB3	1.72	0.70
3:C:56:THR:HG21	3:C:145:CYS:SG	2.32	0.70
9:I:58:VAL:HG13	9:I:62:ILE:HD12	1.72	0.70
2:B:898:LEU:HD13	2:B:952:VAL:HG11	1.73	0.70
8:H:32:THR:HG22	8:H:33:GLN:H	1.57	0.70
7:G:1:MET:SD	7:G:79:PHE:HD1	2.14	0.70
11:K:68:PHE:HB3	11:K:70:ARG:NH1	2.06	0.70
1:A:526:ASP:HB2	2:B:835:GLN:OE1	1.91	0.70
2:B:464:GLY:O	2:B:477:ALA:HA	1.91	0.70
3:C:239:PRO:HB2	3:C:241:ASP:OD1	1.90	0.70
7:G:34:VAL:HG11	7:G:74:TYR:HE1	1.56	0.70
1:A:35:ILE:CG2	1:A:84:ILE:HD12	2.21	0.70
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:589:VAL:HG12	2:B:590:HIS:N	2.06	0.70
6:F:90:ARG:HG3	6:F:91:ALA:N	2.06	0.70
1:A:84:ILE:HG23	1:A:84:ILE:O	1.92	0.70
2:B:101:MET:HB2	2:B:169:ARG:NH2	2.07	0.70
2:B:824:ILE:HG22	2:B:1087:PHE:CE2	2.27	0.70
8:H:64:ASN:HD22	8:H:88:SER:CB	2.04	0.70
1:A:49:LYS:NZ	1:A:61:ILE:HG13	2.06	0.70
2:B:978:ASP:OD2	2:B:1098:MET:HG2	1.91	0.70
2:B:850:LEU:HD12	2:B:851:PHE:N	2.06	0.70
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.73	0.70
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.27	0.69
2:B:54:PHE:O	2:B:58:THR:HB	1.92	0.69
2:B:60:GLN:HE22	2:B:94:LYS:HA	1.57	0.69
4:D:47:LEU:HD13	4:D:48:ILE:N	2.04	0.69
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.27	0.69
6:F:106:PRO:HB2	6:F:108:PHE:CE2	2.27	0.69
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.72	0.69
1:A:1210:GLY:O	1:A:1214:GLU:HG2	1.92	0.69
1:A:447:GLN:HE22	13:T:20:DG:H4'	1.55	0.69
2:B:465:ASN:N	2:B:465:ASN:ND2	2.40	0.69
3:C:73:GLN:HE21	3:C:75:MET:N	1.89	0.69
1:A:1006:ILE:CD1	5:E:163:GLU:HG3	2.20	0.69
1:A:852:TYR:CD1	6:F:136:ARG:HB3	2.28	0.69
6:F:73:ALA:HB1	6:F:143:PHE:O	1.91	0.69
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.73	0.69
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.87	0.69
1:A:602:ASP:HB3	1:A:616:VAL:HG23	1.74	0.69
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.89	0.69
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.07	0.69
3:C:18:VAL:HG23	3:C:240:VAL:HG12	1.74	0.69
3:C:89:GLU:O	3:C:90:ASP:HB3	1.90	0.69
12:L:60:ARG:HH21	12:L:65:VAL:HG21	1.57	0.69
1:A:1120:LEU:H	1:A:1120:LEU:HD12	1.57	0.69
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.23	0.69
1:A:825:ILE:HG23	1:A:826:ASP:N	2.08	0.69
2:B:243:ALA:HB2	2:B:251:ILE:HG12	1.74	0.69
2:B:465:ASN:HD22	2:B:465:ASN:N	1.89	0.69
2:B:821:GLN:HE22	2:B:851:PHE:N	1.90	0.69
5:E:168:TYR:HB3	5:E:170:LEU:HG	1.74	0.69
1:A:1420:ASP:O	1:A:1421:CYS:HB2	1.93	0.69
1:A:443:LEU:HD23	1:A:501:LEU:CD2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.28	0.69
5:E:124:VAL:HG13	5:E:132:ILE:HG13	1.73	0.69
5:E:190:LEU:HD12	5:E:214:CYS:HB2	1.75	0.69
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.74	0.69
2:B:1202:LEU:O	2:B:1206:GLU:HG3	1.92	0.69
3:C:261:ALA:O	3:C:265:MET:HB2	1.92	0.69
7:G:96:GLN:O	7:G:112:LYS:HD3	1.92	0.69
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.73	0.69
8:H:82:PRO:HG3	11:K:54:ARG:HH11	1.56	0.69
1:A:53:LEU:HD23	1:A:54:ASN:HB3	1.74	0.69
2:B:326:ASP:C	2:B:328:GLU:H	1.95	0.69
7:G:125:SER:OG	7:G:128:PRO:HA	1.92	0.69
8:H:14:GLU:HG2	8:H:15:VAL:N	2.08	0.69
1:A:106:VAL:HG13	1:A:112:LYS:O	1.93	0.69
1:A:596:THR:C	1:A:598:LEU:H	1.97	0.69
1:A:72:GLU:HB3	1:A:76:GLU:HG2	1.75	0.69
2:B:121:ASN:HA	2:B:207:GLY:HA2	1.75	0.69
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.75	0.69
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.75	0.69
1:A:1151:GLU:HG2	9:I:45:ARG:HB2	1.75	0.69
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.93	0.69
1:A:356:ASP:HB2	1:A:469:ARG:HH12	1.58	0.69
1:A:49:LYS:HZ3	1:A:61:ILE:HG13	1.58	0.69
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.74	0.69
2:B:563:MET:CE	2:B:580:VAL:HB	2.23	0.69
2:B:25:ILE:HD11	2:B:653:VAL:O	1.92	0.69
9:I:58:VAL:HG13	9:I:62:ILE:CD1	2.23	0.69
1:A:1032:LEU:O	1:A:1036:ARG:HD3	1.94	0.68
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.74	0.68
1:A:898:ARG:HD2	1:A:899:VAL:N	2.08	0.68
2:B:289:LEU:HD13	2:B:375:ALA:CB	2.23	0.68
2:B:613:VAL:HG13	2:B:627:PHE:O	1.92	0.68
3:C:251:LEU:O	3:C:255:VAL:HG23	1.94	0.68
3:C:36:VAL:HG21	3:C:251:LEU:HD13	1.74	0.68
1:A:567:LYS:CE	8:H:47:PHE:HB2	2.23	0.68
1:A:1208:THR:HB	1:A:1211:GLN:HG3	1.75	0.68
1:A:12:ARG:HD2	2:B:1218:THR:HB	1.73	0.68
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.28	0.68
7:G:119:LEU:HD12	7:G:131:GLN:O	1.93	0.68
1:A:1081:LEU:HD11	1:A:1097:GLY:HA3	1.75	0.68
1:A:1116:LEU:HB3	1:A:1308:THR:HG21	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:PRO:HB3	1:A:428:TYR:HE2	1.56	0.68
1:A:442:VAL:O	1:A:457:ALA:HA	1.92	0.68
1:A:722:LEU:HD23	1:A:799:PHE:CD1	2.28	0.68
5:E:202:SER:OG	5:E:204:THR:HG22	1.94	0.68
2:B:309:GLN:OE1	9:I:52:ILE:HD11	1.93	0.68
1:A:11:LEU:HD12	2:B:1193:GLN:O	1.92	0.68
1:A:1348:LEU:O	1:A:1352:VAL:HG23	1.93	0.68
7:G:44:TYR:HE1	7:G:157:ILE:H	1.40	0.68
1:A:547:LEU:HD22	11:K:58:PHE:CE1	2.28	0.68
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.24	0.68
1:A:1345:ARG:NH1	5:E:200:ARG:HH22	1.92	0.68
1:A:573:SER:O	1:A:576:GLN:HB2	1.93	0.68
2:B:1095:LEU:CD1	2:B:1095:LEU:H	1.96	0.68
2:B:253:THR:HG22	2:B:254:LEU:H	1.58	0.68
2:B:90:ILE:HG23	2:B:133:LYS:O	1.93	0.68
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.74	0.68
4:D:40:HIS:HD2	7:G:73:LYS:HG2	1.57	0.68
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.28	0.68
8:H:109:LYS:HD2	8:H:111:LEU:HD11	1.76	0.68
9:I:99:LEU:O	9:I:111:THR:HG23	1.94	0.68
2:B:620:ARG:NH1	9:I:68:LEU:HD21	2.08	0.68
1:A:741:ASN:HD22	1:A:744:LYS:H	1.42	0.68
1:A:960:ILE:HA	1:A:963:ILE:HG22	1.76	0.68
2:B:1084:GLN:OE1	3:C:189:THR:HG22	1.92	0.68
2:B:1069:PHE:HA	2:B:1085:ILE:O	1.94	0.68
2:B:326:ASP:CG	2:B:328:GLU:HB3	2.14	0.68
3:C:238:ILE:CD1	3:C:246:ARG:HH11	2.07	0.68
3:C:43:THR:CG2	3:C:44:LEU:H	1.95	0.68
11:K:31:VAL:HG12	11:K:32:VAL:N	2.06	0.68
1:A:717:ASN:HA	1:A:720:ARG:NH1	2.09	0.68
2:B:824:ILE:CG2	2:B:1087:PHE:HE2	2.06	0.68
3:C:34:ARG:HA	3:C:37:MET:HE2	1.76	0.68
4:D:47:LEU:O	4:D:48:ILE:HD13	1.92	0.68
5:E:22:MET:HE3	5:E:26:ARG:NH1	2.06	0.68
6:F:84:TYR:CE2	6:F:152:ILE:HD12	2.29	0.68
1:A:1081:LEU:CD1	1:A:1098:VAL:H	2.07	0.68
2:B:1099:VAL:CG1	2:B:1100:ASP:H	2.05	0.68
2:B:219:ALA:HB2	2:B:405:ARG:NH1	2.08	0.68
2:B:563:MET:HE3	2:B:580:VAL:HB	1.76	0.68
6:F:74:ILE:HG23	6:F:75:PRO:HD2	1.75	0.68
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:654:ARG:H	2:B:657:HIS:CD2	2.08	0.67
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.74	0.67
1:A:1308:THR:HG23	1:A:1310:GLY:H	1.59	0.67
1:A:180:LYS:HZ1	1:A:294:SER:HB3	1.57	0.67
1:A:528:LEU:O	1:A:531:ILE:HG22	1.95	0.67
1:A:903:ASN:ND2	1:A:904:THR:N	2.41	0.67
2:B:1224:PHE:CE1	5:E:171:LYS:HG3	2.29	0.67
1:A:1223:ASP:HA	1:A:1243:VAL:HG11	1.76	0.67
1:A:1276:VAL:HG12	1:A:1277:GLU:H	1.58	0.67
1:A:102:VAL:HB	1:A:211:PHE:CZ	2.30	0.67
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.15	0.67
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.28	0.67
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.75	0.67
1:A:709:THR:HG21	9:I:93:LYS:O	1.95	0.67
1:A:33:ALA:HB3	1:A:82:GLY:HA3	1.77	0.67
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.29	0.67
1:A:866:PHE:C	1:A:867:ILE:HD12	2.14	0.67
1:A:129:LYS:O	1:A:130:ASP:HB2	1.93	0.67
3:C:3:GLU:CB	11:K:104:ASN:HD21	2.07	0.67
9:I:71:SER:OG	9:I:83:ASN:HB2	1.93	0.67
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.76	0.67
1:A:732:LEU:O	1:A:736:ASN:HB2	1.95	0.67
2:B:289:LEU:HD13	2:B:375:ALA:HB2	1.76	0.67
2:B:942:ARG:HH22	13:T:23:BRU:H5"	1.58	0.67
1:A:1224:LEU:HD11	1:A:1240:CYS:HB2	1.76	0.67
1:A:1144:LYS:HB2	1:A:1268:LEU:O	1.94	0.67
1:A:265:LYS:HE2	1:A:302:THR:CG2	2.24	0.67
2:B:1174:LYS:O	2:B:1176:ASN:N	2.28	0.67
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.56	0.67
14:N:2:DG:H4'	14:N:3:DT:OP1	1.93	0.67
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.25	0.67
1:A:1175:SER:O	1:A:1176:LEU:HB2	1.94	0.67
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.24	0.67
5:E:136:ASN:O	5:E:140:LEU:HG	1.95	0.67
11:K:21:ILE:HG22	11:K:31:VAL:CG1	2.24	0.67
1:A:335:ARG:CD	2:B:1202:LEU:HD23	2.25	0.67
2:B:1150:ARG:HA	2:B:1154:ALA:HB3	1.77	0.67
2:B:430:ARG:O	2:B:434:ARG:CG	2.43	0.67
1:A:1127:ASP:CG	1:A:1130:GLN:HB2	2.15	0.67
1:A:1372:VAL:O	1:A:1376:THR:HG22	1.95	0.67
1:A:2:VAL:HG11	2:B:1157:ALA:CB	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:HD22	1:A:80:HIS:O	1.95	0.67
1:A:630:ILE:HD11	1:A:646:PHE:HZ	1.60	0.67
1:A:647:GLY:O	1:A:651:LYS:HG3	1.94	0.67
2:B:35:SER:O	2:B:39:ARG:HG3	1.94	0.67
3:C:184:ASN:ND2	3:C:187:LYS:HA	2.09	0.67
7:G:23:LYS:HG3	7:G:56:ILE:CD1	2.24	0.67
2:B:769:TYR:CE1	15:P:11:U:H2'	2.30	0.66
2:B:785:TYR:CE1	2:B:795:ILE:HG12	2.30	0.66
1:A:1052:GLN:HA	1:A:1055:ARG:NH1	2.10	0.66
1:A:284:ALA:C	1:A:286:HIS:H	1.96	0.66
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.24	0.66
1:A:406:ILE:HG13	1:A:431:LYS:HB2	1.75	0.66
1:A:504:LEU:HD11	6:F:91:ALA:HB1	1.77	0.66
1:A:869:GLY:O	5:E:204:THR:HG21	1.95	0.66
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.29	0.66
2:B:294:ASP:O	2:B:296:GLU:N	2.29	0.66
2:B:416:LEU:HD11	2:B:466:TRP:CZ2	2.30	0.66
2:B:999:MET:HE3	2:B:999:MET:HA	1.75	0.66
4:D:117:GLU:O	4:D:118:THR:HG23	1.94	0.66
2:B:102:VAL:HG11	12:L:54:ARG:NH2	2.09	0.66
1:A:873:MET:C	1:A:1058:VAL:HG23	2.16	0.66
1:A:335:ARG:HH11	2:B:1202:LEU:CD2	2.07	0.66
2:B:1215:ARG:C	2:B:1216:LEU:HD23	2.15	0.66
2:B:575:PRO:HG2	2:B:576:ASP:H	1.59	0.66
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.60	0.66
2:B:792:MET:HA	2:B:856:PHE:O	1.96	0.66
8:H:26:ILE:HG22	8:H:27:GLU:N	2.10	0.66
2:B:114:PRO:HG2	2:B:115:GLN:H	1.61	0.66
2:B:639:ILE:HD11	2:B:691:GLU:CG	2.26	0.66
3:C:8:VAL:HG12	3:C:9:LYS:H	1.60	0.66
8:H:125:LEU:HG	8:H:126:GLU:H	1.59	0.66
11:K:53:ASP:HB3	11:K:56:VAL:HG23	1.75	0.66
1:A:1120:LEU:HD22	1:A:1124:HIS:O	1.96	0.66
1:A:310:GLY:O	1:A:312:PRO:HD2	1.94	0.66
7:G:23:LYS:HG3	7:G:56:ILE:HD11	1.78	0.66
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	1.94	0.66
1:A:541:ILE:HD13	1:A:549:MET:CE	2.26	0.66
1:A:746:MET:HE3	2:B:1018:PRO:HG2	1.78	0.66
2:B:1048:THR:OG1	2:B:1050:ILE:HD13	1.96	0.66
2:B:164:LYS:N	2:B:164:LYS:HE2	2.11	0.66
2:B:253:THR:HG22	2:B:254:LEU:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:ILE:HD12	2:B:347:LYS:HE2	1.77	0.66
5:E:156:LEU:HA	5:E:160:GLU:OE1	1.95	0.66
1:A:265:LYS:HD3	1:A:303:TYR:HA	1.76	0.66
2:B:276:ILE:HA	2:B:337:ARG:O	1.95	0.66
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.76	0.66
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.77	0.66
5:E:153:HIS:HB3	5:E:196:VAL:CG1	2.26	0.66
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.60	0.66
9:I:35:VAL:HG12	9:I:36:GLU:N	2.11	0.66
10:J:64:ASN:CB	10:J:65:PRO:CD	2.71	0.66
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.31	0.66
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.77	0.66
3:C:242:GLN:C	3:C:244:VAL:H	1.98	0.66
4:D:32:GLU:OE1	7:G:41:LYS:HE2	1.96	0.66
1:A:832:ALA:HA	13:T:18:DA:C8	2.30	0.66
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.30	0.66
2:B:723:VAL:HG12	2:B:724:ASP:N	2.08	0.66
2:B:934:LYS:CG	2:B:934:LYS:O	2.41	0.66
5:E:55:ARG:C	5:E:57:MET:H	1.99	0.66
9:I:71:SER:HG	9:I:101:PHE:HD2	1.44	0.66
1:A:356:ASP:OD1	1:A:358:ASN:N	2.27	0.65
2:B:1183:LYS:C	2:B:1186:ASP:H	1.99	0.65
2:B:314:LEU:O	2:B:318:VAL:HG23	1.96	0.65
2:B:546:SER:OG	2:B:631:GLY:N	2.27	0.65
2:B:57:TYR:HD1	2:B:57:TYR:H	1.41	0.65
2:B:599:THR:O	2:B:603:LEU:HB2	1.96	0.65
2:B:980:PHE:HE2	2:B:1094:ARG:HB2	1.61	0.65
4:D:134:THR:CG2	4:D:135:GLY:H	2.07	0.65
4:D:53:SER:H	4:D:148:LEU:HD21	1.59	0.65
13:T:9:DC:H2"	13:T:10:DA:H8	1.58	0.65
1:A:1111:MET:HE1	1:A:1331:SER:HA	1.77	0.65
1:A:43:GLU:HG3	1:A:48:ALA:HB3	1.78	0.65
1:A:575:LYS:HD2	8:H:120:GLY:HA2	1.79	0.65
1:A:666:ILE:HD12	1:A:667:GLY:N	2.06	0.65
1:A:528:LEU:HD23	1:A:751:SER:HB3	1.78	0.65
4:D:155:ARG:HG3	4:D:155:ARG:HH11	1.62	0.65
4:D:180:LEU:CD2	4:D:195:ILE:HD12	2.26	0.65
5:E:124:VAL:N	5:E:125:PRO:CD	2.59	0.65
8:H:33:GLN:NE2	8:H:35:GLN:HB2	1.98	0.65
9:I:82:GLU:O	9:I:104:LEU:HG	1.97	0.65
1:A:174:ILE:HG22	1:A:175:ARG:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:TRP:HA	1:A:576:GLN:OE1	1.96	0.65
2:B:778:MET:HE2	2:B:1094:ARG:HG2	1.77	0.65
3:C:176:ILE:HG22	3:C:177:GLU:N	2.11	0.65
4:D:173:HIS:CD2	4:D:174:PRO:HD2	2.31	0.65
8:H:81:PRO:CG	8:H:82:PRO:HD2	2.26	0.65
1:A:12:ARG:O	2:B:1194:ILE:HG22	1.96	0.65
1:A:321:PRO:O	1:A:322:VAL:HG12	1.96	0.65
1:A:541:ILE:HD13	1:A:549:MET:HE3	1.79	0.65
2:B:243:ALA:HA	2:B:250:PHE:O	1.95	0.65
2:B:460:ALA:HB1	2:B:466:TRP:CZ3	2.30	0.65
4:D:137:ASN:HD22	4:D:137:ASN:N	1.94	0.65
4:D:155:ARG:HD3	4:D:221:TYR:CE1	2.32	0.65
9:I:4:PHE:HE1	9:I:6:PHE:HE2	1.43	0.65
1:A:682:THR:CG2	1:A:728:LYS:HE3	2.27	0.65
2:B:708:GLU:HG3	2:B:709:ASP:H	1.61	0.65
2:B:857:ARG:HH21	2:B:942:ARG:NH2	1.92	0.65
8:H:64:ASN:CG	8:H:90:ALA:H	1.99	0.65
10:J:14:VAL:HG12	10:J:14:VAL:O	1.96	0.65
1:A:1424:VAL:HG13	1:A:1436:ILE:CD1	2.20	0.65
3:C:68:GLY:O	3:C:169:LYS:HB2	1.97	0.65
10:J:30:LEU:HD11	10:J:38:ARG:NH1	2.11	0.65
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.61	0.65
1:A:851:HIS:O	1:A:853:ASP:N	2.30	0.65
2:B:1180:PHE:HB3	2:B:1191:ILE:HD12	1.78	0.65
2:B:578:THR:H	2:B:589:VAL:CG1	2.10	0.65
2:B:872:GLU:OE1	2:B:914:LYS:HE3	1.96	0.65
3:C:82:TYR:CZ	3:C:161:LYS:HG2	2.32	0.65
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.32	0.65
2:B:1069:PHE:HD1	2:B:1069:PHE:H	1.44	0.65
1:A:35:ILE:HA	1:A:52:GLY:O	1.97	0.65
1:A:743:VAL:O	1:A:747:VAL:HG23	1.97	0.65
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.26	0.65
2:B:387:LEU:O	2:B:392:ARG:HB2	1.97	0.65
6:F:75:PRO:O	6:F:77:ASP:O	2.15	0.65
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.31	0.65
1:A:1223:ASP:HA	1:A:1243:VAL:CG1	2.27	0.65
1:A:1259:MET:HG3	1:A:1262:LYS:HZ2	1.62	0.65
1:A:306:ASN:ND2	1:A:322:VAL:HG12	2.12	0.65
1:A:332:LYS:HA	1:A:337:ARG:HD2	1.79	0.65
1:A:416:ARG:HG3	1:A:417:TYR:CE2	2.32	0.65
1:A:666:ILE:N	2:B:1026:LEU:HD13	2.08	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:ALA:HA	13:T:18:DA:N7	2.11	0.65
1:A:886:ILE:HG23	1:A:887:GLY:N	2.11	0.65
2:B:172:ILE:HD13	2:B:178:ASN:HD22	1.61	0.65
2:B:25:ILE:HG23	2:B:658:ILE:HD11	1.79	0.65
2:B:999:MET:HE2	2:B:1000:PRO:HD3	1.77	0.65
3:C:39:ALA:O	3:C:164:ALA:HB3	1.97	0.65
4:D:180:LEU:HD21	4:D:198:LEU:HD11	1.79	0.65
7:G:13:LEU:HD23	7:G:14:HIS:N	2.11	0.65
9:I:111:THR:HG22	9:I:112:SER:N	2.12	0.65
1:A:1074:GLU:C	1:A:1076:ALA:H	2.01	0.64
2:B:283:VAL:HG21	2:B:317:CYS:O	1.97	0.64
2:B:999:MET:HG3	2:B:1000:PRO:CD	2.20	0.64
3:C:181:ASP:OD2	3:C:185:LYS:N	2.30	0.64
5:E:114:ASN:O	5:E:115:ASN:CB	2.45	0.64
6:F:118:LEU:O	6:F:118:LEU:HD12	1.97	0.64
8:H:80:ARG:HH11	11:K:57:LEU:HD21	1.62	0.64
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.23	0.64
1:A:356:ASP:HB2	1:A:469:ARG:NH1	2.11	0.64
1:A:384:ASN:O	1:A:386:ASP:N	2.31	0.64
1:A:65:LEU:HD22	1:A:71:GLN:OE1	1.97	0.64
2:B:956:THR:HG22	2:B:957:ASN:H	1.63	0.64
3:C:5:GLY:O	3:C:7:GLN:HG3	1.98	0.64
6:F:79:ARG:HG2	6:F:79:ARG:NH1	2.11	0.64
9:I:50:THR:HG22	9:I:51:ASN:N	2.11	0.64
10:J:2:ILE:CG2	10:J:3:VAL:N	2.59	0.64
11:K:19:LEU:HD22	11:K:33:ILE:HG21	1.79	0.64
11:K:61:TYR:C	11:K:61:TYR:CD2	2.70	0.64
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.32	0.64
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.27	0.64
9:I:76:PRO:HD2	9:I:108:HIS:CD2	2.32	0.64
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.31	0.64
2:B:516:ASN:ND2	2:B:516:ASN:N	2.45	0.64
2:B:854:LEU:O	2:B:855:PHE:HB2	1.96	0.64
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.62	0.64
8:H:42:ILE:HG12	8:H:95:TYR:CE1	2.32	0.64
1:A:1155:ASP:OD2	1:A:1161:THR:HA	1.98	0.64
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.33	0.64
1:A:182:VAL:HG22	1:A:201:VAL:HA	1.78	0.64
1:A:630:ILE:HG23	1:A:631:HIS:N	2.13	0.64
1:A:903:ASN:ND2	1:A:904:THR:H	1.94	0.64
2:B:68:THR:OG1	2:B:91:SER:HB3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:637:LEU:C	2:B:690:VAL:HG13	2.18	0.64
3:C:232:VAL:HG21	3:C:244:VAL:HG22	1.78	0.64
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.32	0.64
2:B:1084:GLN:NE2	2:B:1084:GLN:N	2.46	0.64
1:A:1072:ILE:HD11	1:A:1368:MET:HA	1.80	0.64
1:A:567:LYS:HD3	1:A:568:PRO:HD3	1.80	0.64
2:B:706:GLN:NE2	2:B:730:ARG:HH11	1.94	0.64
1:A:1211:GLN:O	1:A:1214:GLU:HB2	1.98	0.64
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.80	0.64
1:A:68:GLN:O	1:A:70:CYS:N	2.28	0.64
2:B:165:VAL:HG11	2:B:448:ILE:CD1	2.18	0.64
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.78	0.64
3:C:24:ASN:HA	3:C:226:ASP:HB3	1.79	0.64
4:D:68:ARG:O	4:D:72:ARG:HG3	1.98	0.64
1:A:1066:VAL:O	1:A:1070:GLN:HG3	1.98	0.64
1:A:1293:SER:OG	1:A:1295:THR:HG23	1.98	0.64
2:B:53:GLN:HG2	2:B:547:VAL:CG2	2.28	0.64
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.28	0.64
2:B:755:ILE:HG23	2:B:809:MET:CE	2.28	0.64
2:B:882:THR:HG22	2:B:884:ARG:H	1.61	0.64
1:A:1141:THR:OG1	1:A:1205:LYS:HD3	1.97	0.63
1:A:69:THR:C	1:A:71:GLN:N	2.49	0.63
1:A:947:PHE:CE2	1:A:954:TRP:CE2	2.86	0.63
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.80	0.63
3:C:166:GLU:C	11:K:6:ARG:HH11	2.01	0.63
5:E:167:ARG:O	5:E:168:TYR:HD2	1.81	0.63
1:A:1441:PHE:CE2	6:F:89:GLU:HG2	2.34	0.63
1:A:1343:ALA:O	1:A:1346:ALA:HB3	1.97	0.63
1:A:993:LEU:HD23	1:A:1022:LEU:HD11	1.79	0.63
2:B:865:LYS:HD2	2:B:961:LEU:HD21	1.80	0.63
5:E:124:VAL:HG13	5:E:132:ILE:CG1	2.28	0.63
1:A:1404:GLU:HB2	1:A:1408:ILE:CD1	2.29	0.63
2:B:1072:MET:HE3	2:B:1085:ILE:HD13	1.79	0.63
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.80	0.63
2:B:127:GLY:C	2:B:128:LEU:HD12	2.19	0.63
2:B:520:GLY:H	2:B:748:ILE:HG22	1.62	0.63
3:C:66:ARG:HH22	10:J:2:ILE:CG2	2.12	0.63
7:G:106:MET:HG2	7:G:107:LYS:N	2.13	0.63
1:A:1444:MET:HB3	7:G:59:GLY:O	1.97	0.63
3:C:169:LYS:NZ	12:L:69:ALA:HB3	2.12	0.63
1:A:111:GLY:O	1:A:214:ILE:HA	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:LEU:HD13	1:A:1393:ASN:HD22	1.63	0.63
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.80	0.63
1:A:443:LEU:HD11	1:A:455:MET:HB3	1.81	0.63
2:B:806:THR:HG23	2:B:1046:PRO:HD3	1.81	0.63
2:B:130:VAL:HG23	2:B:167:ILE:HD13	1.80	0.63
2:B:363:HIS:O	2:B:364:ILE:HB	1.97	0.63
2:B:955:THR:CG2	2:B:956:THR:N	2.60	0.63
8:H:100:THR:HG22	8:H:101:ALA:N	2.14	0.63
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.79	0.63
1:A:76:GLU:O	1:A:78:PRO:HD3	1.98	0.63
1:A:986:ILE:HD12	1:A:1032:LEU:HD11	1.80	0.63
2:B:53:GLN:HG2	2:B:547:VAL:HG23	1.79	0.63
2:B:785:TYR:HA	2:B:788:ARG:HG3	1.80	0.63
3:C:112:ASN:HB2	3:C:114:TYR:HE1	1.63	0.63
4:D:40:HIS:HB2	7:G:73:LYS:HD3	1.80	0.63
9:I:4:PHE:CD1	9:I:4:PHE:C	2.70	0.63
10:J:7:CYS:O	10:J:11:GLY:HA2	1.97	0.63
1:A:1260:LEU:HD12	1:A:1260:LEU:O	1.97	0.63
1:A:1115:SER:C	1:A:1308:THR:HG22	2.19	0.63
2:B:1050:ILE:N	2:B:1050:ILE:HD12	2.14	0.63
2:B:558:LEU:C	2:B:560:GLU:H	2.01	0.63
2:B:860:MET:HG2	2:B:861:ASP:N	2.12	0.63
7:G:28:THR:O	7:G:32:GLU:HG3	1.98	0.63
8:H:89:LEU:O	8:H:91:ASP:N	2.29	0.63
1:A:825:ILE:CG2	1:A:826:ASP:N	2.61	0.63
2:B:469:GLN:CG	2:B:470:LYS:H	2.11	0.63
2:B:810:GLU:HA	2:B:815:ARG:HH12	1.64	0.63
2:B:847:ASP:C	2:B:849:GLY:H	2.02	0.63
5:E:106:GLN:HA	5:E:130:ALA:CB	2.29	0.63
1:A:1276:VAL:HG12	1:A:1277:GLU:N	2.14	0.63
1:A:103:CYS:SG	1:A:207:ILE:HD12	2.39	0.63
2:B:593:PRO:HA	2:B:596:LEU:HB3	1.81	0.63
3:C:241:ASP:O	3:C:245:VAL:HG23	1.99	0.63
5:E:128:PRO:HA	5:E:129:PRO:O	1.99	0.63
5:E:15:ALA:O	5:E:19:VAL:HG23	1.99	0.63
1:A:1152:ILE:HD11	9:I:44:TYR:HD2	1.63	0.63
1:A:767:GLN:HB2	1:A:799:PHE:HD1	1.64	0.63
2:B:123:THR:O	2:B:125:SER:N	2.32	0.63
2:B:527:THR:OG1	2:B:528:PRO:HD2	1.99	0.63
2:B:615:MET:HB3	2:B:626:ILE:HG12	1.80	0.63
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.78	0.63
4:D:66:ARG:HD2	4:D:133:THR:HB	1.80	0.63
5:E:100:ILE:O	5:E:100:ILE:HG22	1.99	0.63
2:B:186:GLU:CG	10:J:62:ARG:HH22	2.05	0.63
8:H:82:PRO:HG3	11:K:54:ARG:HD2	1.81	0.63
1:A:913:LEU:HD12	1:A:914:GLU:H	1.62	0.62
2:B:579:ARG:HH11	2:B:579:ARG:HG2	1.64	0.62
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.28	0.62
2:B:847:ASP:OD2	3:C:167:HIS:HD2	1.82	0.62
1:A:504:LEU:HD11	6:F:91:ALA:CB	2.29	0.62
10:J:64:ASN:ND2	10:J:65:PRO:HD3	2.14	0.62
1:A:1158:PRO:HB2	1:A:1188:GLN:HE22	1.64	0.62
1:A:35:ILE:HD12	1:A:241:VAL:HG21	1.81	0.62
1:A:590:ARG:HB3	1:A:605:MET:N	2.13	0.62
1:A:523:ILE:HD12	1:A:622:VAL:HG21	1.82	0.62
1:A:814:PHE:CE1	2:B:519:TRP:HA	2.34	0.62
2:B:878:GLN:O	2:B:934:LYS:HE2	1.99	0.62
7:G:143:ILE:CG2	7:G:144:ARG:N	2.62	0.62
8:H:84:ALA:CB	8:H:87:ARG:HD2	2.29	0.62
9:I:50:THR:HG22	9:I:51:ASN:H	1.64	0.62
12:L:61:THR:HG21	12:L:63:ARG:NE	2.14	0.62
1:A:25:GLU:OE1	1:A:25:GLU:N	2.32	0.62
1:A:474:VAL:HA	1:A:521:MET:HE2	1.81	0.62
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.32	0.62
2:B:281:PRO:O	2:B:283:VAL:N	2.33	0.62
9:I:17:ARG:HG3	9:I:28:GLU:OE1	1.99	0.62
11:K:42:LEU:HD23	11:K:42:LEU:C	2.19	0.62
1:A:1017:LEU:HB2	5:E:206:GLY:N	2.00	0.62
1:A:1412:ALA:HA	1:A:1417:GLU:OE2	1.99	0.62
1:A:768:GLN:CG	1:A:816:HIS:HA	2.23	0.62
1:A:902:LEU:HD11	1:A:923:LEU:HD21	1.79	0.62
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.81	0.62
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.35	0.62
7:G:114:LEU:HG	7:G:162:SER:HB3	1.81	0.62
1:A:1340:GLY:O	1:A:1342:GLU:N	2.32	0.62
1:A:754:SER:N	1:A:757:ASN:HD22	1.96	0.62
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.35	0.62
2:B:244:LEU:HD21	2:B:366:GLN:NE2	2.14	0.62
3:C:132:PRO:O	3:C:134:ILE:HG13	2.00	0.62
3:C:6:PRO:HB3	3:C:25:VAL:HG12	1.82	0.62
13:T:21:DC:H2''	13:T:22:DC:C5'	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1279:ILE:O	1:A:1279:ILE:HG22	1.99	0.62
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.14	0.62
1:A:115:LEU:CD1	1:A:141:LEU:HB3	2.30	0.62
1:A:259:GLU:OE1	1:A:263:THR:HG21	1.99	0.62
1:A:427:GLN:HB2	1:A:430:TRP:CD2	2.34	0.62
1:A:50:ILE:O	1:A:52:GLY:N	2.33	0.62
2:B:1002:THR:HG21	2:B:1006:ILE:HG13	1.80	0.62
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.81	0.62
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.81	0.62
7:G:1:MET:SD	7:G:79:PHE:CD1	2.92	0.62
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.29	0.62
1:A:1293:SER:HB2	1:A:1299:VAL:HG23	1.82	0.62
1:A:1445:ILE:H	1:A:1445:ILE:CD1	1.99	0.62
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.82	0.62
2:B:1115:THR:O	2:B:1116:ARG:HB2	1.99	0.62
2:B:244:LEU:HD13	2:B:247:GLY:O	2.00	0.62
1:A:255:SER:OG	2:B:918:ILE:HG21	1.98	0.62
5:E:138:ALA:HA	5:E:141:VAL:HG23	1.82	0.62
5:E:31:THR:CG2	5:E:34:GLU:HB2	2.29	0.62
5:E:54:GLN:O	5:E:57:MET:HB3	1.99	0.62
8:H:93:TYR:HB3	8:H:144:ILE:O	2.00	0.62
13:T:10:DA:H2''	13:T:11:DA:H8	1.61	0.62
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.64	0.62
1:A:463:ILE:HD11	1:A:469:ARG:HG3	1.82	0.62
1:A:606:LEU:HG	1:A:613:ILE:HD12	1.81	0.62
1:A:857:ARG:NH2	6:F:139:PRO:HG3	2.14	0.62
2:B:20:ASP:C	2:B:22:SER:H	2.01	0.62
2:B:331:LEU:HD23	2:B:353:LYS:HG2	1.81	0.62
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.29	0.62
4:D:59:ILE:O	4:D:63:LEU:HB2	2.00	0.62
6:F:103:MET:O	6:F:104:ASN:HB2	2.00	0.62
12:L:53:HIS:HB3	12:L:55:ILE:CD1	2.30	0.62
13:T:24:DG:H2'	13:T:25:DG:H8	1.65	0.62
1:A:438:ASP:OD1	1:A:462:VAL:HG23	2.00	0.62
1:A:744:LYS:O	1:A:748:MET:HG3	2.00	0.62
1:A:834:THR:HG21	1:A:1077:THR:HG23	1.81	0.62
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.80	0.62
2:B:211:VAL:CG2	2:B:483:LEU:HB2	2.29	0.62
2:B:276:ILE:HD13	2:B:280:ILE:HD11	1.82	0.62
1:A:1140:HIS:HA	1:A:1275:GLY:HA3	1.82	0.62
2:B:521:LEU:HD13	2:B:633:VAL:HB	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:THR:HG22	3:C:101:LEU:H	1.64	0.62
3:C:258:ILE:HD11	11:K:42:LEU:HD11	1.81	0.62
7:G:1:MET:SD	7:G:2:PHE:N	2.72	0.62
8:H:109:LYS:HD2	8:H:111:LEU:CD1	2.30	0.62
10:J:48:ARG:NE	10:J:49:MET:HE2	2.08	0.62
12:L:34:CYS:SG	12:L:34:CYS:O	2.58	0.62
1:A:335:ARG:O	1:A:339:ASN:HB2	1.99	0.61
1:A:954:TRP:HB3	1:A:955:PRO:HD2	1.82	0.61
2:B:838:SER:HB2	2:B:989:THR:O	1.99	0.61
3:C:124:LEU:O	3:C:127:ARG:HG2	2.00	0.61
11:K:7:PHE:O	11:K:11:LEU:HD23	1.99	0.61
1:A:1160:SER:HA	1:A:1170:ILE:CD1	2.28	0.61
1:A:335:ARG:HD2	2:B:1202:LEU:HD23	1.82	0.61
2:B:167:ILE:HD12	2:B:167:ILE:N	2.14	0.61
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.36	0.61
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.15	0.61
9:I:78:CYS:O	9:I:80:SER:N	2.32	0.61
2:B:193:LYS:HZ1	12:L:32:ALA:HB1	1.65	0.61
1:A:1187:GLN:HG3	1:A:1188:GLN:N	2.15	0.61
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.46	0.61
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.82	0.61
2:B:611:PRO:CG	2:B:685:LEU:HD21	2.27	0.61
4:D:118:THR:OG1	4:D:121:LYS:HB2	2.00	0.61
6:F:103:MET:HE2	7:G:66:GLY:N	2.14	0.61
11:K:93:SER:O	11:K:97:LYS:HG3	2.00	0.61
1:A:184:SER:HB3	1:A:199:LEU:HD23	1.83	0.61
1:A:93:VAL:HG23	1:A:304:MET:HE3	1.82	0.61
2:B:1215:ARG:O	2:B:1216:LEU:HD23	2.00	0.61
4:D:13:ARG:O	4:D:13:ARG:HD3	1.99	0.61
1:A:224:PHE:CE2	1:A:231:PRO:HG3	2.35	0.61
1:A:40:THR:HB	1:A:41:MET:CE	2.30	0.61
1:A:65:LEU:O	1:A:71:GLN:HA	2.00	0.61
1:A:68:GLN:C	1:A:70:CYS:H	2.04	0.61
2:B:882:THR:HG22	2:B:884:ARG:CB	2.26	0.61
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.81	0.61
6:F:85:MET:O	6:F:155:LEU:HD21	2.00	0.61
6:F:77:ASP:O	6:F:78:GLN:HB2	2.01	0.61
8:H:32:THR:HG22	8:H:33:GLN:N	2.15	0.61
1:A:67:CYS:O	1:A:68:GLN:HB2	2.00	0.61
1:A:744:LYS:HG2	1:A:748:MET:CE	2.31	0.61
2:B:860:MET:HG3	2:B:965:LYS:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1214:GLU:OE1	1:A:1214:GLU:HA	2.00	0.61
1:A:18:GLN:HG2	1:A:1418:LEU:HD13	1.83	0.61
1:A:93:VAL:HG21	1:A:301:ALA:O	2.01	0.61
2:B:20:ASP:O	2:B:22:SER:N	2.30	0.61
2:B:485:ARG:NH2	2:B:782:LEU:HD11	2.16	0.61
2:B:25:ILE:HD11	2:B:653:VAL:C	2.20	0.61
2:B:766:ARG:NH1	2:B:766:ARG:HG2	2.15	0.61
2:B:842:ASN:HD22	2:B:845:SER:CB	2.10	0.61
3:C:112:ASN:HB2	3:C:114:TYR:CE1	2.36	0.61
7:G:30:LEU:HD13	7:G:72:VAL:HG11	1.83	0.61
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.82	0.61
8:H:81:PRO:CB	8:H:82:PRO:CD	2.77	0.61
3:C:50:GLU:HG2	12:L:64:LEU:HD22	1.82	0.61
1:A:1308:THR:HG21	1:A:1310:GLY:O	2.01	0.61
1:A:825:ILE:HD11	2:B:512:ARG:CB	2.31	0.61
2:B:169:ARG:HB3	2:B:169:ARG:HH11	1.65	0.61
2:B:604:ARG:C	2:B:606:LYS:H	2.03	0.61
2:B:980:PHE:CE2	2:B:1094:ARG:HB2	2.34	0.61
3:C:22:LEU:HD13	3:C:230:MET:HE3	1.83	0.61
1:A:1420:ASP:CB	1:A:1422:ARG:HG3	2.22	0.61
1:A:332:LYS:H	1:A:337:ARG:CB	2.13	0.61
1:A:531:ILE:CD1	1:A:653:VAL:HG21	2.30	0.61
1:A:858:ASN:C	1:A:858:ASN:HD22	2.04	0.61
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.83	0.61
3:C:58:LEU:HD22	3:C:58:LEU:N	2.16	0.61
5:E:69:ILE:HA	5:E:72:PHE:O	2.01	0.61
7:G:145:VAL:HG12	7:G:146:LYS:N	2.15	0.61
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.36	0.61
8:H:12:VAL:HB	8:H:52:GLN:N	2.15	0.61
1:A:1213:GLY:HA2	1:A:1216:ILE:HG13	1.82	0.61
1:A:438:ASP:OD2	1:A:461:LYS:HD2	2.00	0.61
1:A:726:ARG:O	1:A:729:ALA:HB3	2.00	0.61
7:G:49:LEU:HG	7:G:76:ALA:HA	1.82	0.61
1:A:560:ILE:CD1	8:H:79:TRP:H	2.12	0.61
12:L:49:LYS:O	12:L:50:ASP:HB2	1.99	0.61
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.83	0.60
1:A:30:ILE:HG23	2:B:1170:THR:CG2	2.30	0.60
2:B:180:TYR:HD1	2:B:180:TYR:H	1.48	0.60
2:B:190:TYR:CE1	2:B:196:PRO:HG3	2.36	0.60
2:B:244:LEU:O	2:B:249:ARG:HG2	2.01	0.60
2:B:591:ARG:O	2:B:593:PRO:HD3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:193:TYR:CD2	3:C:197:SER:HB3	2.35	0.60
1:A:1343:ALA:CB	5:E:150:VAL:HG22	2.30	0.60
5:E:173:SER:O	5:E:175:LEU:N	2.33	0.60
7:G:39:THR:HG22	7:G:41:LYS:H	1.66	0.60
7:G:7:LEU:HB2	7:G:74:TYR:HE2	1.64	0.60
8:H:40:LEU:HD22	8:H:123:MET:HE1	1.83	0.60
9:I:4:PHE:HD1	9:I:4:PHE:C	2.04	0.60
1:A:1114:PRO:C	1:A:1330:ASN:HD21	2.05	0.60
1:A:1258:HIS:HB3	1:A:1259:MET:HE3	1.83	0.60
1:A:418:SER:O	1:A:420:ARG:N	2.28	0.60
1:A:709:THR:HB	1:A:712:GLU:H	1.65	0.60
1:A:885:THR:O	1:A:885:THR:HG22	2.01	0.60
2:B:571:PRO:HG2	2:B:572:HIS:ND1	2.15	0.60
5:E:44:ALA:O	5:E:45:LYS:HB2	2.00	0.60
1:A:299:HIS:HA	1:A:302:THR:HG22	1.81	0.60
1:A:340:LEU:HD21	2:B:1199:ALA:HB3	1.83	0.60
1:A:809:THR:HG23	1:A:812:GLU:OE1	2.00	0.60
1:A:996:ASN:O	1:A:998:LEU:HD12	2.02	0.60
1:A:666:ILE:HD11	2:B:1067:ARG:O	2.01	0.60
2:B:193:LYS:HZ3	12:L:32:ALA:HB1	1.67	0.60
2:B:57:TYR:CD1	2:B:57:TYR:N	2.70	0.60
2:B:485:ARG:CZ	2:B:782:LEU:HD11	2.31	0.60
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.31	0.60
5:E:179:GLN:HB2	5:E:182:ASP:HB2	1.83	0.60
1:A:1244:ARG:CB	1:A:1245:PRO:HA	2.14	0.60
1:A:313:GLN:O	1:A:314:ALA:C	2.40	0.60
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.37	0.60
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.65	0.60
1:A:71:GLN:CG	1:A:72:GLU:N	2.64	0.60
2:B:273:LEU:HD12	2:B:280:ILE:HD12	1.83	0.60
3:C:46:ILE:CG2	3:C:157:CYS:HB3	2.31	0.60
3:C:261:ALA:HA	3:C:264:GLN:OE1	2.02	0.60
6:F:106:PRO:HB2	6:F:108:PHE:HE2	1.66	0.60
7:G:146:LYS:HB2	7:G:168:LEU:HD11	1.83	0.60
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.37	0.60
1:A:523:ILE:HG23	1:A:527:THR:HB	1.83	0.60
1:A:55:ASP:C	1:A:57:ARG:N	2.55	0.60
1:A:69:THR:O	1:A:71:GLN:N	2.34	0.60
2:B:850:LEU:HD12	2:B:851:PHE:H	1.67	0.60
5:E:111:VAL:HG12	5:E:137:GLU:HG2	1.83	0.60
5:E:42:PHE:HZ	5:E:58:MET:HE1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:103:MET:CE	7:G:66:GLY:N	2.63	0.60
11:K:47:ARG:HH11	11:K:47:ARG:CB	2.13	0.60
1:A:1220:PHE:CE2	1:A:1263:ILE:HG23	2.36	0.60
1:A:1424:VAL:O	1:A:1428:VAL:HG23	2.00	0.60
1:A:1445:ILE:HD12	1:A:1445:ILE:N	2.09	0.60
1:A:87:ALA:HB2	1:A:273:ASN:OD1	2.02	0.60
1:A:524:VAL:CG1	1:A:525:GLN:H	2.15	0.60
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.01	0.60
1:A:925:LEU:HD13	1:A:983:ILE:HD12	1.84	0.60
2:B:1097:HIS:N	2:B:1098:MET:HE2	2.16	0.60
2:B:288:ALA:HA	2:B:331:LEU:CD1	2.32	0.60
2:B:467:GLY:O	2:B:469:GLN:N	2.35	0.60
2:B:766:ARG:HG3	2:B:1022:THR:HG23	1.82	0.60
3:C:102:GLN:HG2	3:C:154:LYS:HG2	1.82	0.60
3:C:107:SER:C	3:C:109:SER:H	2.03	0.60
12:L:61:THR:HG22	12:L:63:ARG:N	2.08	0.60
1:A:186:LYS:O	1:A:187:LYS:HB3	2.01	0.60
1:A:280:GLU:C	1:A:282:ASN:H	2.04	0.60
2:B:1000:PRO:O	2:B:1007:VAL:HG23	2.02	0.60
2:B:1186:ASP:O	4:D:17:LYS:HE2	2.01	0.60
2:B:190:TYR:HD2	10:J:62:ARG:O	1.85	0.60
2:B:258:LEU:HG	2:B:258:LEU:O	2.02	0.60
2:B:393:LYS:HA	2:B:393:LYS:HE3	1.83	0.60
2:B:603:LEU:HD13	2:B:608:ASP:HB3	1.82	0.60
3:C:13:ALA:O	11:K:114:LEU:HD22	2.01	0.60
9:I:7:CYS:HB2	9:I:34:TYR:CD2	2.37	0.60
1:A:105:CYS:O	1:A:114:LEU:HG	2.02	0.60
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.82	0.60
1:A:401:GLY:C	1:A:435:HIS:HD2	2.05	0.60
1:A:993:LEU:CD2	1:A:1022:LEU:HD11	2.32	0.60
2:B:638:PHE:HA	2:B:690:VAL:CG2	2.20	0.60
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.83	0.60
2:B:882:THR:O	2:B:883:LEU:HB2	2.02	0.60
1:A:567:LYS:HD2	8:H:95:TYR:CG	2.36	0.60
12:L:38:LEU:HD23	12:L:56:LEU:HD21	1.84	0.60
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.37	0.60
1:A:282:ASN:O	1:A:284:ALA:N	2.35	0.60
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.83	0.60
1:A:542:GLU:HG3	1:A:544:ASP:OD1	2.02	0.60
1:A:590:ARG:HG3	1:A:590:ARG:NH1	2.17	0.60
1:A:918:GLU:HG3	1:A:918:GLU:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:ALA:N	2:B:231:PRO:CD	2.64	0.60
2:B:327:ARG:O	2:B:331:LEU:HD13	2.01	0.60
2:B:641:GLU:HB2	2:B:643:ASP:OD2	2.02	0.60
2:B:882:THR:CG2	2:B:935:ARG:HA	2.32	0.60
2:B:95:ILE:CB	2:B:130:VAL:HG22	2.31	0.60
3:C:236:GLY:O	3:C:238:ILE:N	2.35	0.60
4:D:22:GLU:H	4:D:22:GLU:CD	2.05	0.60
6:F:89:GLU:O	6:F:93:ILE:HG13	2.01	0.60
12:L:27:LEU:N	12:L:27:LEU:HD23	2.16	0.60
1:A:1063:MET:SD	1:A:1436:ILE:HG23	2.42	0.60
1:A:1081:LEU:CD1	1:A:1098:VAL:HG23	2.32	0.60
1:A:12:ARG:CZ	2:B:1192:TYR:HE2	2.15	0.60
1:A:262:LEU:HD21	1:A:303:TYR:CE1	2.36	0.60
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.83	0.60
5:E:17:ARG:CB	5:E:17:ARG:HH11	2.14	0.60
7:G:91:VAL:HG23	7:G:141:SER:O	2.02	0.60
8:H:104:PHE:CE2	8:H:136:LYS:HG2	2.37	0.60
9:I:58:VAL:HG12	9:I:58:VAL:O	1.99	0.60
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.15	0.59
1:A:276:LEU:HD13	1:A:293:GLU:HA	1.83	0.59
1:A:93:VAL:CG2	1:A:304:MET:HE3	2.32	0.59
1:A:471:ASN:OD1	1:A:472:LEU:N	2.35	0.59
2:B:365:THR:OG1	2:B:367:LEU:HG	2.02	0.59
4:D:123:LEU:HD11	4:D:150:ASN:OD1	2.02	0.59
5:E:100:ILE:CG2	5:E:105:PHE:HB2	2.31	0.59
7:G:6:ASP:HB3	7:G:73:LYS:HZ1	1.66	0.59
8:H:139:ASN:O	8:H:140:ALA:HB2	2.02	0.59
10:J:1:MET:N	10:J:56:LEU:HB2	2.17	0.59
1:A:1315:GLU:O	1:A:1317:MET:N	2.35	0.59
1:A:248:PRO:O	1:A:260:ASP:HB2	2.02	0.59
1:A:322:VAL:CG1	1:A:322:VAL:O	2.50	0.59
1:A:92:HIS:CD2	1:A:304:MET:HE1	2.37	0.59
2:B:596:LEU:O	2:B:600:LEU:HG	2.02	0.59
2:B:870:ILE:HG22	2:B:917:PRO:HG2	1.83	0.59
3:C:18:VAL:HG12	3:C:18:VAL:O	2.02	0.59
4:D:170:THR:CG2	4:D:172:LEU:HG	2.32	0.59
8:H:81:PRO:HB2	8:H:82:PRO:HD2	1.84	0.59
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.33	0.59
1:A:1315:GLU:C	1:A:1317:MET:N	2.55	0.59
1:A:865:GLN:HE21	1:A:1370:LEU:HA	1.67	0.59
1:A:19:PHE:O	1:A:1416:ALA:HA	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:VAL:C	1:A:228:PHE:HD2	2.05	0.59
1:A:24:PRO:HB3	1:A:237:THR:HB	1.84	0.59
1:A:56:PRO:O	1:A:57:ARG:HG3	2.03	0.59
1:A:49:LYS:NZ	1:A:61:ILE:N	2.41	0.59
1:A:12:ARG:HB2	2:B:1218:THR:CG2	2.32	0.59
2:B:51:PHE:O	2:B:55:VAL:HG23	2.02	0.59
2:B:638:PHE:CB	2:B:651:LEU:HD22	2.32	0.59
5:E:55:ARG:C	5:E:57:MET:N	2.55	0.59
8:H:12:VAL:HB	8:H:52:GLN:H	1.66	0.59
1:A:1116:LEU:HD13	1:A:1329:THR:HB	1.84	0.59
1:A:524:VAL:CG1	1:A:525:GLN:N	2.64	0.59
1:A:55:ASP:N	1:A:56:PRO:HD3	2.16	0.59
2:B:446:LEU:O	2:B:447:ALA:HB3	2.03	0.59
2:B:821:GLN:HE22	2:B:850:LEU:HD12	1.66	0.59
3:C:36:VAL:CG2	3:C:251:LEU:HD13	2.32	0.59
4:D:137:ASN:N	4:D:137:ASN:ND2	2.48	0.59
4:D:71:LYS:HA	4:D:74:GLN:CG	2.32	0.59
5:E:180:ARG:NH2	5:E:192:ARG:HD2	2.18	0.59
7:G:138:THR:HG22	7:G:139:ILE:HG13	1.83	0.59
4:D:40:HIS:HB2	7:G:73:LYS:NZ	2.17	0.59
2:B:955:THR:OG1	12:L:55:ILE:HA	2.03	0.59
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.37	0.59
1:A:434:ARG:HH11	1:A:434:ARG:HG2	1.68	0.59
1:A:62:ASP:O	1:A:63:ARG:C	2.41	0.59
1:A:341:MET:CE	1:A:843:LYS:NZ	2.66	0.59
2:B:555:ILE:HD11	2:B:587:HIS:CE1	2.38	0.59
2:B:658:ILE:HG22	2:B:662:MET:HE2	1.84	0.59
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.84	0.59
1:A:1373:ASP:HA	1:A:1376:THR:CG2	2.32	0.59
1:A:1402:PHE:O	1:A:1403:GLU:HB2	2.03	0.59
1:A:172:PRO:HG3	1:A:185:TRP:CZ2	2.38	0.59
1:A:645:LEU:O	1:A:649:ILE:HG13	2.02	0.59
1:A:466:SER:O	2:B:1103:ILE:HD11	2.02	0.59
2:B:579:ARG:N	2:B:589:VAL:HG13	2.17	0.59
3:C:166:GLU:HB3	3:C:170:TRP:HZ3	1.67	0.59
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.84	0.59
3:C:88:CYS:SG	3:C:91:HIS:C	2.80	0.59
4:D:52:LEU:HD12	4:D:182:SER:HB2	1.83	0.59
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	1.83	0.59
5:E:198:ILE:HD12	5:E:198:ILE:N	2.18	0.59
12:L:55:ILE:O	12:L:56:LEU:CB	2.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1290:LYS:O	1:A:1291:VAL:HG23	2.02	0.59
1:A:1313:LEU:O	1:A:1315:GLU:N	2.35	0.59
1:A:1345:ARG:NH1	5:E:200:ARG:NH2	2.50	0.59
1:A:233:TRP:C	1:A:235:ILE:H	2.04	0.59
1:A:37:PHE:N	1:A:37:PHE:CD1	2.68	0.59
2:B:1040:ASN:O	2:B:1042:GLY:N	2.35	0.59
2:B:383:ASN:C	2:B:387:LEU:HD13	2.22	0.59
2:B:410:GLY:HA2	2:B:413:LEU:HD12	1.85	0.59
2:B:597:MET:HA	2:B:597:MET:CE	2.33	0.59
2:B:853:SER:O	2:B:854:LEU:HD23	2.02	0.59
3:C:137:LYS:HB2	3:C:138:GLU:OE1	2.03	0.59
8:H:118:PHE:O	8:H:120:GLY:N	2.35	0.59
11:K:18:LYS:NZ	11:K:38:GLU:HG2	2.17	0.59
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.68	0.59
1:A:1377:THR:OG1	1:A:1378:GLN:N	2.36	0.59
1:A:445:ASN:CB	1:A:455:MET:HG2	2.32	0.59
1:A:590:ARG:O	1:A:591:PHE:HB2	2.02	0.59
1:A:825:ILE:HD11	2:B:512:ARG:CD	2.31	0.59
2:B:175:ARG:HH11	2:B:175:ARG:HG2	1.67	0.59
2:B:174:LEU:HD22	2:B:202:TYR:CE1	2.37	0.59
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.33	0.59
3:C:93:ASP:OD1	3:C:122:SER:HB2	2.03	0.59
5:E:198:ILE:HD11	5:E:212:ARG:HB2	1.85	0.59
8:H:44:VAL:HG12	8:H:44:VAL:O	2.03	0.59
9:I:102:VAL:HA	9:I:108:HIS:O	2.03	0.59
3:C:165:LYS:O	11:K:6:ARG:NH1	2.36	0.59
1:A:468:PHE:CZ	1:A:489:LEU:HD23	2.37	0.59
1:A:477:PRO:HG2	1:A:521:MET:CE	2.33	0.59
1:A:541:ILE:N	1:A:572:TRP:O	2.35	0.59
1:A:466:SER:HB2	2:B:1099:VAL:CG2	2.33	0.59
2:B:188:ASP:O	2:B:192:LEU:HD12	2.02	0.59
4:D:204:ASP:O	4:D:208:GLU:HB2	2.02	0.59
2:B:1006:ILE:HD13	10:J:44:TYR:CE2	2.37	0.59
11:K:102:LYS:O	11:K:106:GLU:HG3	2.03	0.59
12:L:26:THR:HG23	12:L:62:LYS:HZ1	1.66	0.59
1:A:1404:GLU:CB	1:A:1408:ILE:HG13	2.33	0.59
1:A:346:ASP:OD1	2:B:1108:ARG:HA	2.02	0.59
1:A:531:ILE:HD12	1:A:653:VAL:HG21	1.83	0.59
1:A:898:ARG:HD3	1:A:933:TYR:CD1	2.37	0.59
2:B:642:ASP:CA	2:B:649:LYS:HG3	2.33	0.59
2:B:773:MET:CE	2:B:985:GLY:HA2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:LYS:NZ	3:C:194:GLU:HA	2.18	0.59
4:D:49:ALA:HB1	4:D:178:ALA:HB2	1.84	0.59
9:I:6:PHE:HD1	9:I:11:ASN:OD1	1.86	0.59
3:C:169:LYS:HZ3	12:L:69:ALA:HB3	1.67	0.59
1:A:1057:VAL:CG1	1:A:1058:VAL:H	2.14	0.58
1:A:1146:VAL:HG11	1:A:1207:LEU:HD12	1.86	0.58
1:A:219:PHE:CD2	1:A:231:PRO:HD2	2.37	0.58
1:A:323:LYS:N	1:A:323:LYS:HD2	2.17	0.58
1:A:848:ILE:HA	1:A:857:ARG:O	2.03	0.58
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.33	0.58
3:C:186:LEU:HD21	3:C:224:GLN:O	2.04	0.58
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.83	0.58
11:K:23:PRO:HA	11:K:31:VAL:HG13	1.83	0.58
11:K:45:LEU:HG	11:K:94:ILE:CD1	2.32	0.58
1:A:233:TRP:C	1:A:235:ILE:N	2.55	0.58
1:A:40:THR:HB	1:A:41:MET:HE2	1.85	0.58
1:A:56:PRO:O	1:A:57:ARG:CG	2.51	0.58
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.38	0.58
2:B:839:MET:HG3	2:B:1010:LEU:HD11	1.83	0.58
1:A:345:VAL:HG21	2:B:1150:ARG:NH2	2.17	0.58
2:B:335:GLY:CA	2:B:348:ARG:HB2	2.32	0.58
2:B:582:VAL:HG22	2:B:626:ILE:CG2	2.33	0.58
10:J:44:TYR:CD2	10:J:44:TYR:N	2.68	0.58
12:L:30:ILE:HD11	12:L:59:ALA:HB2	1.85	0.58
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.84	0.58
1:A:1107:VAL:HG12	1:A:1107:VAL:O	2.03	0.58
1:A:845:LEU:CD2	1:A:1374:VAL:HG21	2.33	0.58
1:A:41:MET:HE3	1:A:41:MET:H	1.68	0.58
2:B:1002:THR:HG21	2:B:1006:ILE:CD1	2.33	0.58
2:B:1178:ASN:O	2:B:1179:GLN:C	2.42	0.58
2:B:336:ARG:HE	2:B:348:ARG:NH1	2.00	0.58
2:B:781:PHE:HE2	2:B:793:ALA:HB1	1.69	0.58
3:C:107:SER:O	3:C:109:SER:N	2.30	0.58
4:D:40:HIS:CB	7:G:73:LYS:NZ	2.65	0.58
3:C:167:HIS:CE1	12:L:70:ARG:HA	2.38	0.58
1:A:107:CYS:H	1:A:114:LEU:HD21	1.69	0.58
1:A:567:LYS:CG	1:A:568:PRO:HD3	2.34	0.58
2:B:171:PRO:HD2	2:B:457:LEU:CD1	2.33	0.58
2:B:622:LYS:HE2	9:I:59:VAL:CG2	2.31	0.58
2:B:519:TRP:HE1	2:B:635:ARG:NH2	2.02	0.58
2:B:811:TYR:N	2:B:811:TYR:CD1	2.70	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:105:GLY:HA3	3:C:148:ARG:O	2.02	0.58
8:H:129:TYR:H	8:H:130:ARG:HH11	1.52	0.58
8:H:23:VAL:HG22	8:H:43:ASN:HA	1.85	0.58
9:I:13:MET:CE	9:I:14:LEU:H	2.16	0.58
1:A:450:LEU:HD13	1:A:1074:GLU:HG2	1.84	0.58
1:A:506:ALA:HB1	1:A:508:PRO:HD2	1.85	0.58
1:A:69:THR:C	1:A:71:GLN:H	2.05	0.58
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.69	0.58
2:B:121:ASN:HA	2:B:207:GLY:CA	2.34	0.58
2:B:654:ARG:N	2:B:657:HIS:HD2	1.97	0.58
2:B:65:GLU:HG3	2:B:66:ASP:N	2.18	0.58
3:C:166:GLU:HB3	3:C:170:TRP:CZ3	2.38	0.58
3:C:238:ILE:HG22	3:C:243:VAL:HG23	1.85	0.58
14:N:4:DA:H2"	14:N:5:DC:C6	2.39	0.58
1:A:332:LYS:HG3	1:A:333:GLU:HG2	1.85	0.58
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.39	0.58
2:B:1222:ARG:O	2:B:1223:ASP:HB2	2.03	0.58
2:B:648:HIS:CG	2:B:649:LYS:H	2.20	0.58
2:B:120:ARG:HE	2:B:955:THR:HG21	1.68	0.58
3:C:173:ALA:O	3:C:174:ALA:CB	2.52	0.58
3:C:80:LEU:HD11	3:C:95:CYS:C	2.24	0.58
4:D:167:LEU:O	4:D:170:THR:OG1	2.21	0.58
10:J:23:ASN:O	10:J:25:LEU:N	2.36	0.58
10:J:1:MET:H1	10:J:57:ILE:N	2.01	0.58
3:C:3:GLU:HG3	11:K:104:ASN:OD1	2.03	0.58
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.33	0.58
1:A:1201:ALA:O	1:A:1203:ASN:N	2.35	0.58
1:A:115:LEU:O	1:A:122:MET:HG2	2.04	0.58
1:A:212:LYS:HG2	1:A:232:GLU:HB2	1.85	0.58
1:A:243:PRO:HB2	1:A:244:PRO:HD2	1.86	0.58
1:A:332:LYS:N	1:A:337:ARG:HB3	2.19	0.58
1:A:396:PRO:HB3	1:A:403:LYS:HA	1.84	0.58
2:B:115:GLN:HG2	2:B:193:LYS:CB	2.30	0.58
2:B:857:ARG:NH2	2:B:942:ARG:CZ	2.67	0.58
6:F:147:SER:OG	6:F:150:GLU:HG3	2.04	0.58
7:G:34:VAL:HG11	7:G:74:TYR:CE1	2.37	0.58
8:H:4:THR:HA	8:H:60:ALA:HB2	1.85	0.58
12:L:68:GLU:CD	12:L:68:GLU:H	2.07	0.58
1:A:20:GLY:O	1:A:21:LEU:HD23	2.04	0.58
1:A:619:LYS:HD2	1:A:750:GLY:O	2.04	0.58
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:LYS:HG2	3:C:15:LYS:O	2.03	0.58
3:C:174:ALA:O	3:C:175:ALA:HB2	2.04	0.58
3:C:243:VAL:HG12	3:C:243:VAL:O	2.03	0.58
4:D:130:LEU:O	4:D:132:GLN:N	2.35	0.58
1:A:1227:ILE:CG2	1:A:1228:TRP:H	2.12	0.58
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.33	0.58
1:A:385:ILE:HG22	1:A:386:ASP:N	2.18	0.58
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.85	0.58
1:A:590:ARG:HH11	1:A:590:ARG:CG	2.17	0.58
1:A:596:THR:O	1:A:598:LEU:N	2.33	0.58
2:B:229:ALA:CB	2:B:231:PRO:HD2	2.33	0.58
2:B:331:LEU:CD2	2:B:353:LYS:HG2	2.33	0.58
10:J:48:ARG:C	10:J:48:ARG:HD2	2.23	0.58
13:T:11:DA:H2"	13:T:12:DG:H8	1.69	0.58
1:A:115:LEU:HG	1:A:142:CYS:HB3	1.85	0.58
2:B:284:ILE:HD13	2:B:333:PHE:CD2	2.39	0.58
2:B:639:ILE:CG2	2:B:641:GLU:HG2	2.34	0.58
2:B:842:ASN:ND2	2:B:845:SER:HB3	2.14	0.58
2:B:866:TYR:HD1	2:B:870:ILE:O	1.86	0.58
3:C:100:THR:HG22	3:C:101:LEU:N	2.19	0.58
3:C:174:ALA:O	10:J:10:CYS:O	2.22	0.58
2:B:1065:GLN:HB2	3:C:201:TRP:CZ3	2.39	0.58
2:B:1084:GLN:HG2	3:C:201:TRP:HZ2	1.66	0.58
4:D:25:ALA:C	4:D:27:LEU:H	2.06	0.58
6:F:152:ILE:HG22	6:F:153:VAL:H	1.68	0.58
8:H:15:VAL:HG22	8:H:26:ILE:HD13	1.85	0.58
1:A:447:GLN:NE2	13:T:20:DG:H4'	2.19	0.58
1:A:1377:THR:O	1:A:1379:GLY:N	2.36	0.57
1:A:306:ASN:HD22	1:A:322:VAL:HG12	1.68	0.57
1:A:794:PRO:HG2	1:A:795:GLU:OE2	2.03	0.57
2:B:801:LYS:N	10:J:52:THR:HG23	2.18	0.57
6:F:79:ARG:HG2	6:F:79:ARG:HH11	1.69	0.57
1:A:341:MET:HE3	1:A:843:LYS:HZ1	1.68	0.57
2:B:133:LYS:HE3	2:B:135:ARG:HH21	1.70	0.57
2:B:181:LEU:HD23	2:B:189:LEU:HD22	1.86	0.57
2:B:31:TRP:CE3	2:B:31:TRP:HA	2.39	0.57
2:B:351:TYR:CZ	2:B:355:ILE:HD11	2.39	0.57
2:B:508:LEU:O	2:B:509:ALA:HB2	2.03	0.57
2:B:975:GLN:O	2:B:990:ILE:HD12	2.04	0.57
4:D:153:ARG:HB3	4:D:154:PHE:CD1	2.39	0.57
5:E:111:VAL:CG1	5:E:137:GLU:HG2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:99:HIS:CE1	5:E:103:LYS:HG3	2.39	0.57
6:F:111:LEU:N	6:F:111:LEU:HD12	2.15	0.57
8:H:100:THR:HG23	8:H:138:GLU:CA	2.33	0.57
9:I:100:PHE:N	9:I:100:PHE:HD1	2.02	0.57
1:A:477:PRO:HG2	1:A:521:MET:HE2	1.85	0.57
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.39	0.57
2:B:570:VAL:HG21	2:B:573:GLN:HB3	1.85	0.57
8:H:14:GLU:O	8:H:26:ILE:HG23	2.03	0.57
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.34	0.57
1:A:1213:GLY:HA2	1:A:1216:ILE:CG1	2.34	0.57
1:A:1394:THR:CG2	1:A:1398:MET:SD	2.92	0.57
1:A:79:GLY:CA	1:A:243:PRO:HG3	2.34	0.57
1:A:372:LYS:HA	1:A:435:HIS:CE1	2.38	0.57
1:A:709:THR:HG22	1:A:710:LEU:N	2.19	0.57
1:A:729:ALA:HA	1:A:732:LEU:HD12	1.87	0.57
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.39	0.57
2:B:498:THR:O	2:B:536:VAL:HA	2.05	0.57
2:B:997:GLU:H	2:B:997:GLU:CD	2.08	0.57
8:H:127:GLY:O	8:H:128:ASN:HB2	2.04	0.57
1:A:1152:ILE:CD1	9:I:44:TYR:HD2	2.17	0.57
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.37	0.57
1:A:1187:GLN:HG3	1:A:1188:GLN:H	1.68	0.57
1:A:53:LEU:CD2	1:A:54:ASN:HB3	2.34	0.57
1:A:740:LEU:HD12	1:A:741:ASN:N	2.20	0.57
2:B:278:GLN:HG2	2:B:279:ASP:H	1.69	0.57
2:B:309:GLN:O	2:B:312:GLU:HB3	2.04	0.57
2:B:333:PHE:CE1	2:B:337:ARG:NH2	2.73	0.57
4:D:24:ALA:C	4:D:26:THR:N	2.58	0.57
1:A:1100:ARG:HH12	1:A:1111:MET:HE3	1.68	0.57
1:A:1284:MET:O	1:A:1285:MET:HG2	2.04	0.57
1:A:469:ARG:HB3	1:A:469:ARG:NH1	2.19	0.57
2:B:1200:ALA:HA	2:B:1203:LEU:HB3	1.87	0.57
2:B:899:ILE:HD11	2:B:910:VAL:O	2.05	0.57
6:F:111:LEU:H	6:F:111:LEU:CD1	2.13	0.57
7:G:116:PRO:HG2	7:G:119:LEU:HB2	1.86	0.57
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.86	0.57
10:J:24:LEU:HA	10:J:28:ASP:HB2	1.86	0.57
1:A:537:ARG:HH12	8:H:122:LEU:HG	1.70	0.57
1:A:335:ARG:HH11	2:B:1202:LEU:HD23	1.68	0.57
2:B:167:ILE:HG22	2:B:453:ILE:CD1	2.33	0.57
1:A:786:HIS:HE1	2:B:519:TRP:CZ2	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:589:VAL:HG12	2:B:590:HIS:H	1.69	0.57
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.35	0.57
3:C:58:LEU:CD2	3:C:58:LEU:H	2.18	0.57
6:F:70:LYS:C	6:F:72:LYS:H	2.07	0.57
7:G:153:GLN:O	7:G:154:VAL:C	2.42	0.57
7:G:59:GLY:HA3	7:G:70:PHE:CD2	2.39	0.57
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.37	0.57
11:K:6:ARG:O	11:K:9:LEU:HG	2.05	0.57
1:A:1103:GLU:O	1:A:1108:ALA:HB2	2.05	0.57
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.05	0.57
1:A:567:LYS:HZ3	8:H:95:TYR:CB	2.18	0.57
1:A:594:GLY:H	1:A:603:ASN:ND2	2.02	0.57
1:A:774:ARG:NH2	1:A:797:LYS:HB2	2.19	0.57
1:A:913:LEU:HD11	1:A:981:LEU:O	2.04	0.57
1:A:341:MET:HE1	2:B:1135:ARG:NH1	2.19	0.57
3:C:123:ASN:CG	3:C:125:MET:H	2.08	0.57
6:F:86:THR:HG23	6:F:89:GLU:OE1	2.04	0.57
7:G:119:LEU:HD12	7:G:132:SER:HB2	1.86	0.57
8:H:125:LEU:HG	8:H:126:GLU:N	2.20	0.57
11:K:63:VAL:O	11:K:63:VAL:HG23	2.05	0.57
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.05	0.57
1:A:1258:HIS:HB3	1:A:1259:MET:CE	2.35	0.57
1:A:409:SER:O	1:A:411:ASP:N	2.38	0.57
1:A:808:LEU:HD23	1:A:813:PHE:CA	2.33	0.57
1:A:947:PHE:CD1	1:A:947:PHE:N	2.73	0.57
2:B:601:ARG:HD3	2:B:605:ARG:HH21	1.69	0.57
2:B:638:PHE:HB3	2:B:651:LEU:HD22	1.87	0.57
3:C:241:ASP:O	3:C:244:VAL:HB	2.04	0.57
5:E:182:ASP:O	5:E:185:ALA:HB3	2.05	0.57
5:E:17:ARG:O	5:E:21:GLU:HG3	2.04	0.57
9:I:69:PRO:HG2	9:I:85:PHE:CD2	2.39	0.57
10:J:1:MET:N	10:J:56:LEU:N	2.53	0.57
1:A:1005:GLU:HG3	1:A:1006:ILE:N	2.19	0.57
1:A:108:MET:HA	1:A:210:ILE:CG2	2.35	0.57
2:B:181:LEU:HD23	2:B:189:LEU:CD2	2.35	0.57
2:B:635:ARG:HB2	2:B:636:PRO:HD2	1.86	0.57
2:B:882:THR:C	2:B:884:ARG:H	2.09	0.57
4:D:51:ASN:OD1	4:D:54:GLU:HB3	2.05	0.57
5:E:144:ILE:HG13	5:E:145:THR:H	1.69	0.57
12:L:26:THR:HG22	12:L:27:LEU:N	2.20	0.57
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1146:PHE:CE1	2:B:1150:ARG:HD3	2.39	0.56
2:B:299:GLU:HG2	2:B:571:PRO:HG3	1.87	0.56
2:B:594:ALA:HA	2:B:617:ARG:NH1	2.18	0.56
3:C:25:VAL:HG22	3:C:228:PHE:HE1	1.70	0.56
1:A:564:ALA:O	8:H:97:MET:HA	2.05	0.56
1:A:32:VAL:HG21	1:A:68:GLN:HE22	1.70	0.56
1:A:340:LEU:CD2	2:B:1199:ALA:HB3	2.36	0.56
1:A:52:GLY:O	1:A:56:PRO:HG2	2.05	0.56
1:A:899:VAL:HG13	1:A:908:LEU:HD21	1.87	0.56
2:B:615:MET:HA	2:B:625:LYS:O	2.05	0.56
2:B:980:PHE:HD2	2:B:1094:ARG:HA	1.70	0.56
3:C:242:GLN:C	3:C:244:VAL:N	2.58	0.56
3:C:2:SER:O	3:C:3:GLU:HB2	2.06	0.56
6:F:103:MET:HE1	7:G:66:GLY:H	1.69	0.56
7:G:79:PHE:HZ	7:G:106:MET:HE2	1.70	0.56
10:J:2:ILE:O	10:J:53:HIS:NE2	2.38	0.56
3:C:51:VAL:HB	12:L:65:VAL:HG23	1.85	0.56
1:A:150:THR:O	1:A:150:THR:HG22	2.05	0.56
1:A:186:LYS:O	1:A:194:ALA:HB1	2.05	0.56
1:A:252:PHE:O	1:A:256:GLN:HB2	2.06	0.56
1:A:446:ARG:HB2	1:A:487:MET:SD	2.45	0.56
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.69	0.56
1:A:979:SER:OG	1:A:980:ASP:N	2.37	0.56
1:A:78:PRO:HB2	2:B:1201:LYS:HE3	1.87	0.56
2:B:364:ILE:CG1	2:B:585:VAL:HG13	2.33	0.56
5:E:180:ARG:HB2	5:E:215:MET:OXT	2.04	0.56
5:E:9:ILE:HD11	5:E:53:PRO:HD3	1.85	0.56
7:G:85:GLU:HB3	7:G:147:ILE:HD12	1.87	0.56
8:H:64:ASN:HD22	8:H:88:SER:HB2	1.68	0.56
10:J:36:LEU:HB2	10:J:47:ARG:NH1	2.20	0.56
1:A:427:GLN:HB2	1:A:430:TRP:CD1	2.39	0.56
1:A:889:SER:HA	1:A:1297:GLU:N	2.21	0.56
1:A:947:PHE:N	1:A:947:PHE:HD1	2.02	0.56
2:B:686:ASN:C	2:B:688:GLY:H	2.09	0.56
3:C:101:LEU:C	3:C:102:GLN:HG3	2.26	0.56
3:C:73:GLN:HB3	3:C:131:HIS:H	1.70	0.56
3:C:66:ARG:NH1	10:J:2:ILE:CG2	2.56	0.56
7:G:9:LEU:HD12	7:G:10:ASN:H	1.70	0.56
13:T:15:DC:H2"	13:T:16:DT:C7	2.33	0.56
1:A:1042:PHE:CE2	1:A:1046:LEU:HD11	2.41	0.56
1:A:22:PHE:HE2	1:A:30:ILE:HD12	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:HG12	1:A:297:GLN:NE2	2.21	0.56
1:A:767:GLN:OE1	1:A:799:PHE:HB2	2.04	0.56
1:A:871:ASP:OD2	1:A:873:MET:HB2	2.06	0.56
2:B:224:GLN:NE2	2:B:403:LYS:HD3	2.20	0.56
10:J:27:GLU:C	10:J:29:GLU:H	2.08	0.56
1:A:358:ASN:ND2	2:B:833:TYR:OH	2.39	0.56
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.86	0.56
1:A:717:ASN:HA	1:A:720:ARG:HH12	1.70	0.56
1:A:818:MET:HA	2:B:514:LEU:HB3	1.88	0.56
1:A:466:SER:HB2	2:B:1099:VAL:HG21	1.87	0.56
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.36	0.56
2:B:365:THR:HG23	2:B:367:LEU:H	1.70	0.56
2:B:766:ARG:HH11	2:B:766:ARG:HG2	1.70	0.56
3:C:112:ASN:CB	3:C:114:TYR:CE1	2.89	0.56
3:C:57:VAL:HG11	10:J:60:PHE:CB	2.31	0.56
5:E:171:LYS:HG2	5:E:174:GLN:OE1	2.06	0.56
6:F:138:LEU:O	6:F:140:ASP:N	2.38	0.56
7:G:48:VAL:HA	7:G:76:ALA:HB2	1.86	0.56
3:C:167:HIS:HA	11:K:6:ARG:HH12	1.71	0.56
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.69	0.56
1:A:860:LEU:CD1	1:A:1393:ASN:HD22	2.18	0.56
1:A:353:ILE:CD1	1:A:487:MET:HE2	2.36	0.56
1:A:341:MET:CE	1:A:843:LYS:HZ1	2.18	0.56
1:A:341:MET:HE3	1:A:843:LYS:NZ	2.20	0.56
1:A:986:ILE:CD1	1:A:1032:LEU:HD11	2.36	0.56
2:B:562:GLY:HA3	2:B:590:HIS:ND1	2.20	0.56
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.87	0.56
3:C:213:PRO:HG2	3:C:214:ASN:H	1.71	0.56
4:D:130:LEU:C	4:D:132:GLN:H	2.08	0.56
4:D:50:LEU:HD11	7:G:4:ILE:HD11	1.88	0.56
7:G:14:HIS:ND1	7:G:15:PRO:HD2	2.20	0.56
1:A:1259:MET:C	1:A:1261:LYS:H	2.09	0.56
1:A:41:MET:SD	1:A:42:ASP:N	2.78	0.56
1:A:583:PRO:HG2	1:A:586:ILE:HG13	1.87	0.56
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.36	0.56
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.35	0.56
2:B:1159:ARG:NE	2:B:1193:GLN:HE21	2.04	0.56
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.71	0.56
2:B:652:LYS:O	2:B:689:LEU:HD22	2.05	0.56
1:A:244:PRO:HG2	1:A:245:PRO:HD3	1.86	0.56
1:A:560:ILE:HD11	8:H:79:TRP:N	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:123:ASN:HD21	3:C:125:MET:HA	1.70	0.56
3:C:11:ARG:H	3:C:20:PHE:HA	1.69	0.56
4:D:118:THR:CG2	4:D:121:LYS:HD2	2.32	0.56
4:D:27:LEU:HD22	4:D:173:HIS:ND1	2.21	0.56
5:E:145:THR:HG21	5:E:187:TYR:CD2	2.41	0.56
1:A:1019:CYS:O	1:A:1022:LEU:HB3	2.05	0.56
1:A:427:GLN:HB2	1:A:430:TRP:CG	2.40	0.56
1:A:446:ARG:HB3	1:A:478:TYR:HB3	1.88	0.56
1:A:993:LEU:HD22	1:A:1046:LEU:CD2	2.36	0.56
2:B:294:ASP:C	2:B:296:GLU:H	2.09	0.56
2:B:309:GLN:CD	9:I:52:ILE:HD11	2.26	0.56
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.87	0.56
5:E:144:ILE:HG13	5:E:145:THR:N	2.20	0.56
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.87	0.56
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.45	0.56
1:A:1198:ASP:HB3	1:A:1201:ALA:CB	2.35	0.56
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.06	0.56
1:A:901:LEU:N	1:A:926:GLN:NE2	2.43	0.56
2:B:29:ASP:CG	2:B:658:ILE:HD13	2.25	0.56
2:B:32:ALA:O	2:B:35:SER:HB2	2.05	0.56
2:B:555:ILE:HG22	2:B:556:THR:N	2.19	0.56
2:B:405:ARG:HA	2:B:631:GLY:O	2.06	0.56
5:E:124:VAL:H	5:E:125:PRO:HD2	1.69	0.56
5:E:156:LEU:HD12	5:E:195:VAL:CB	2.33	0.56
8:H:111:LEU:HA	8:H:127:GLY:O	2.06	0.56
1:A:1009:ASN:HA	1:A:1012:ARG:HH11	1.68	0.55
1:A:116:ASP:C	1:A:118:HIS:N	2.55	0.55
1:A:1120:LEU:HD11	1:A:1304:TRP:O	2.05	0.55
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.41	0.55
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.28	0.55
1:A:696:GLU:OE2	1:A:702:LEU:HD21	2.06	0.55
2:B:844:SER:O	2:B:847:ASP:HB2	2.05	0.55
8:H:102:TYR:OH	8:H:122:LEU:HD22	2.06	0.55
1:A:567:LYS:HZ2	8:H:95:TYR:N	2.04	0.55
1:A:1107:VAL:CG2	1:A:1383:SER:HB3	2.36	0.55
1:A:613:ILE:O	1:A:614:PHE:HB3	2.04	0.55
1:A:960:ILE:O	1:A:963:ILE:HG22	2.06	0.55
2:B:1192:TYR:CD2	2:B:1218:THR:HG21	2.41	0.55
2:B:510:LYS:CB	2:B:511:PRO:HD3	2.36	0.55
3:C:42:PRO:HB3	3:C:161:LYS:HE3	1.89	0.55
4:D:156:ASP:HB3	4:D:159:THR:OG1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:136:ARG:O	6:F:143:PHE:CB	2.52	0.55
8:H:102:TYR:N	8:H:102:TYR:CD2	2.68	0.55
9:I:100:PHE:CD1	9:I:100:PHE:N	2.72	0.55
3:C:66:ARG:CZ	10:J:2:ILE:HG21	2.34	0.55
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.36	0.55
13:T:19:8OG:N3	13:T:19:8OG:H2"	2.20	0.55
1:A:1267:MET:O	1:A:1271:ILE:HB	2.07	0.55
1:A:189:ARG:O	1:A:190:ALA:HB3	2.06	0.55
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.40	0.55
2:B:102:VAL:O	2:B:102:VAL:HG12	2.06	0.55
2:B:542:MET:HG2	2:B:747:MET:CE	2.36	0.55
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.36	0.55
2:B:773:MET:SD	2:B:987:LYS:HG2	2.46	0.55
2:B:873:THR:O	2:B:914:LYS:HA	2.05	0.55
2:B:770:GLN:CD	2:B:983:ARG:HA	2.27	0.55
5:E:98:ILE:O	5:E:102:GLU:HG3	2.07	0.55
5:E:109:ILE:HG22	5:E:110:PHE:N	2.21	0.55
12:L:53:HIS:O	12:L:55:ILE:HD13	2.07	0.55
1:A:606:LEU:HB3	1:A:614:PHE:CD2	2.42	0.55
1:A:675:THR:O	1:A:679:ILE:HG13	2.07	0.55
1:A:825:ILE:CG2	1:A:826:ASP:H	2.18	0.55
2:B:785:TYR:CD1	2:B:795:ILE:HG12	2.42	0.55
5:E:23:VAL:HG13	5:E:78:LEU:CD1	2.36	0.55
5:E:78:LEU:HD23	5:E:79:TRP:N	2.21	0.55
1:A:511:ILE:HG21	1:A:634:THR:HG21	1.87	0.55
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.71	0.55
3:C:100:THR:HG22	3:C:102:GLN:HE21	1.71	0.55
3:C:73:GLN:NE2	3:C:74:SER:H	2.04	0.55
9:I:95:THR:HG22	9:I:96:SER:O	2.07	0.55
12:L:38:LEU:CD1	12:L:49:LYS:HG2	2.36	0.55
1:A:1030:ARG:HG3	1:A:1034:GLU:CD	2.27	0.55
1:A:1161:THR:C	1:A:1163:ILE:H	2.08	0.55
1:A:144:THR:O	1:A:146:MET:HG3	2.07	0.55
1:A:845:LEU:O	1:A:846:GLU:C	2.45	0.55
2:B:243:ALA:CB	2:B:251:ILE:HG12	2.36	0.55
2:B:345:LYS:HA	2:B:348:ARG:HG2	1.88	0.55
2:B:289:LEU:HD22	2:B:371:GLU:O	2.07	0.55
2:B:616:ILE:CD1	2:B:625:LYS:HB2	2.36	0.55
3:C:50:GLU:HG2	3:C:50:GLU:O	2.06	0.55
5:E:167:ARG:O	5:E:168:TYR:CD2	2.60	0.55
9:I:85:PHE:N	9:I:85:PHE:CD2	2.63	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:79:GLU:HG3	11:K:80:GLY:H	1.72	0.55
1:A:1057:VAL:CG1	1:A:1058:VAL:N	2.70	0.55
1:A:108:MET:HB3	1:A:210:ILE:CD1	2.27	0.55
2:B:590:HIS:CD2	2:B:596:LEU:HD22	2.42	0.55
10:J:23:ASN:C	10:J:25:LEU:N	2.59	0.55
13:T:18:DA:OP1	13:T:18:DA:H3'	2.06	0.55
13:T:7:DC:H2''	13:T:8:DT:C7	2.36	0.55
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.69	0.55
1:A:34:LYS:HB3	1:A:36:ARG:HH21	1.72	0.55
1:A:381:THR:CG2	1:A:382:PRO:HD2	2.37	0.55
1:A:496:GLU:O	1:A:499:ALA:HB3	2.06	0.55
1:A:506:ALA:HB3	1:A:509:LEU:HD12	1.88	0.55
1:A:512:VAL:HA	1:A:519:PRO:HA	1.88	0.55
2:B:999:MET:HE2	2:B:1000:PRO:CD	2.37	0.55
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.87	0.55
4:D:138:ASN:HD21	7:G:35:GLU:HB3	1.71	0.55
5:E:103:LYS:HB3	5:E:105:PHE:CE2	2.42	0.55
4:D:40:HIS:HB2	7:G:73:LYS:CD	2.37	0.55
11:K:79:GLU:HG3	11:K:80:GLY:N	2.22	0.55
12:L:43:THR:O	12:L:43:THR:HG22	2.07	0.55
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.46	0.55
1:A:1130:GLN:HG3	1:A:1134:ILE:CD1	2.36	0.55
1:A:1272:THR:C	1:A:1273:LEU:HD12	2.27	0.55
1:A:1341:ILE:O	1:A:1344:GLY:N	2.40	0.55
1:A:1396:ALA:HA	1:A:1399:ARG:NH2	2.22	0.55
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.29	0.55
1:A:470:LEU:CD2	1:A:470:LEU:H	2.18	0.55
2:B:1159:ARG:HE	2:B:1193:GLN:HE21	1.54	0.55
2:B:565:PRO:O	2:B:567:GLU:N	2.39	0.55
3:C:175:ALA:HB2	10:J:10:CYS:CB	2.37	0.55
5:E:117:THR:HG22	5:E:119:SER:N	2.14	0.55
5:E:13:TRP:CZ3	5:E:39:LEU:HB2	2.41	0.55
6:F:108:PHE:HE1	6:F:131:PRO:HG3	1.72	0.55
7:G:17:PHE:N	7:G:17:PHE:CD2	2.74	0.55
9:I:109:ILE:HG22	9:I:109:ILE:O	2.07	0.55
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.42	0.55
1:A:267:ALA:O	1:A:271:LYS:HG3	2.06	0.55
2:B:839:MET:HG3	2:B:1010:LEU:CD1	2.37	0.55
2:B:1122:ARG:HB3	13:T:22:DC:OP1	2.06	0.55
2:B:217:ARG:C	2:B:217:ARG:HD2	2.27	0.55
2:B:343:ILE:O	2:B:345:LYS:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:449:ASN:O	2:B:451:LYS:N	2.40	0.55
2:B:562:GLY:O	2:B:590:HIS:ND1	2.38	0.55
2:B:570:VAL:CG2	2:B:573:GLN:HB3	2.37	0.55
2:B:948:ILE:CD1	12:L:67:PHE:HE2	2.20	0.55
3:C:7:GLN:HG2	11:K:104:ASN:HD22	1.72	0.55
1:A:1404:GLU:HB2	1:A:1408:ILE:HG13	1.88	0.54
1:A:18:GLN:NE2	1:A:228:PHE:CE1	2.75	0.54
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.43	0.54
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.72	0.54
2:B:1063:GLY:O	3:C:202:PRO:HG2	2.07	0.54
2:B:776:GLN:O	2:B:1095:LEU:HB3	2.07	0.54
2:B:378:LEU:HD12	2:B:378:LEU:O	2.07	0.54
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.88	0.54
2:B:515:HIS:CD2	2:B:517:THR:H	2.14	0.54
2:B:696:GLU:O	2:B:699:GLU:HB2	2.06	0.54
2:B:857:ARG:HH21	2:B:942:ARG:CZ	2.20	0.54
2:B:898:LEU:HD13	2:B:952:VAL:CG1	2.36	0.54
9:I:6:PHE:N	9:I:6:PHE:CD2	2.71	0.54
2:B:1031:LEU:HA	2:B:1055:ILE:HD13	1.90	0.54
2:B:488:TYR:CE2	2:B:813:LYS:HB2	2.42	0.54
2:B:520:GLY:N	2:B:748:ILE:HG22	2.22	0.54
2:B:405:ARG:NE	2:B:629:ASP:OD2	2.37	0.54
1:A:567:LYS:HZ3	8:H:95:TYR:HB2	1.71	0.54
9:I:106:CYS:O	9:I:107:SER:HB2	2.05	0.54
2:B:1038:SER:O	10:J:33:GLY:HA3	2.07	0.54
1:A:1028:THR:O	1:A:1032:LEU:HD12	2.07	0.54
1:A:1054:LEU:O	1:A:1057:VAL:HG23	2.07	0.54
1:A:1158:PRO:O	1:A:1159:ARG:HG2	2.08	0.54
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.36	0.54
1:A:279:LEU:HB3	1:A:289:ILE:HG12	1.89	0.54
1:A:548:ASN:HA	11:K:60:ALA:HB1	1.90	0.54
2:B:284:ILE:HG23	2:B:324:ILE:CD1	2.36	0.54
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.42	0.54
2:B:906:SER:HA	2:B:946:ASN:HB2	1.90	0.54
2:B:953:LEU:HD23	2:B:965:LYS:O	2.07	0.54
4:D:70:PHE:O	4:D:74:GLN:HG3	2.07	0.54
5:E:52:ARG:HB3	5:E:53:PRO:CD	2.38	0.54
8:H:82:PRO:HG3	11:K:54:ARG:NH1	2.23	0.54
1:A:1389:PHE:C	1:A:1389:PHE:CD1	2.80	0.54
1:A:233:TRP:O	1:A:235:ILE:N	2.40	0.54
1:A:418:SER:C	1:A:420:ARG:H	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:HB2	1:A:247:ARG:HH12	1.73	0.54
2:B:1182:CYS:O	2:B:1183:LYS:O	2.24	0.54
2:B:326:ASP:C	2:B:328:GLU:N	2.61	0.54
3:C:13:ALA:O	11:K:114:LEU:HD13	2.06	0.54
3:C:148:ARG:HG2	3:C:149:LYS:H	1.71	0.54
7:G:47:CYS:O	7:G:76:ALA:HB1	2.07	0.54
8:H:11:GLN:O	8:H:28:ALA:HB1	2.08	0.54
2:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.88	0.54
2:B:948:ILE:HD11	12:L:67:PHE:HE2	1.73	0.54
1:A:963:ILE:HD13	1:A:1049:ILE:CG1	2.36	0.54
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.41	0.54
2:B:1049:ASP:C	2:B:1050:ILE:HD12	2.28	0.54
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.89	0.54
2:B:648:HIS:CG	2:B:649:LYS:N	2.76	0.54
2:B:65:GLU:HG3	2:B:66:ASP:OD1	2.06	0.54
5:E:129:PRO:O	5:E:130:ALA:C	2.46	0.54
5:E:124:VAL:HA	5:E:132:ILE:CD1	2.36	0.54
9:I:99:LEU:C	9:I:100:PHE:HD1	2.10	0.54
9:I:35:VAL:HG12	9:I:36:GLU:H	1.71	0.54
1:A:254:GLU:HB2	2:B:935:ARG:NH2	2.22	0.54
1:A:663:SER:OG	1:A:664:THR:N	2.40	0.54
1:A:711:ARG:O	1:A:714:PHE:HB3	2.07	0.54
2:B:388:CYS:C	2:B:390:LEU:N	2.59	0.54
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.38	0.54
3:C:147:LEU:HD23	3:C:147:LEU:N	2.23	0.54
3:C:43:THR:O	3:C:77:ILE:HG13	2.08	0.54
11:K:27:ALA:HB1	11:K:28:PRO:HD2	1.90	0.54
1:A:1370:LEU:O	1:A:1373:ASP:HB2	2.08	0.54
1:A:383:TYR:N	1:A:383:TYR:CD2	2.74	0.54
1:A:61:ILE:HG22	1:A:62:ASP:H	1.73	0.54
1:A:630:ILE:HD11	1:A:646:PHE:CZ	2.43	0.54
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.43	0.54
7:G:49:LEU:CD2	7:G:77:VAL:HG23	2.21	0.54
7:G:88:ASP:HB3	7:G:144:ARG:CB	2.38	0.54
2:B:266:ALA:O	2:B:268:THR:HG22	2.08	0.54
2:B:215:GLN:OE1	2:B:479:VAL:HG22	2.07	0.54
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.89	0.54
7:G:88:ASP:HB3	7:G:144:ARG:CA	2.36	0.54
8:H:82:PRO:O	8:H:84:ALA:N	2.38	0.54
1:A:1151:GLU:HG2	9:I:45:ARG:CB	2.37	0.54
10:J:2:ILE:HG22	10:J:3:VAL:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:32:GLU:CD	10:J:32:GLU:H	2.11	0.54
14:N:6:DT:H2"	14:N:7:DT:OP2	2.06	0.54
1:A:1158:PRO:CB	1:A:1188:GLN:HE22	2.20	0.54
1:A:193:ASP:O	1:A:194:ALA:HB3	2.08	0.54
1:A:783:THR:HG21	1:A:815:PHE:CZ	2.42	0.54
1:A:488:ASN:OD1	2:B:1128:LEU:HD13	2.08	0.54
1:A:345:VAL:HG21	2:B:1150:ARG:HH22	1.73	0.54
4:D:60:LYS:CE	4:D:126:ILE:HD11	2.38	0.54
6:F:70:LYS:O	6:F:72:LYS:HD2	2.08	0.54
11:K:53:ASP:OD1	11:K:55:LYS:HB2	2.07	0.54
12:L:30:ILE:HG22	12:L:31:CYS:H	1.71	0.54
15:P:3:U:H2'	15:P:4:C:C6	2.43	0.54
1:A:1015:VAL:O	1:A:1017:LEU:N	2.41	0.54
1:A:1104:ILE:HG21	1:A:1352:VAL:HG22	1.90	0.54
1:A:24:PRO:HD3	1:A:233:TRP:CD1	2.42	0.54
1:A:41:MET:O	1:A:42:ASP:O	2.26	0.54
1:A:456:MET:HE2	1:A:507:VAL:HA	1.89	0.54
1:A:567:LYS:HG2	1:A:568:PRO:N	2.23	0.54
1:A:741:ASN:ND2	1:A:744:LYS:N	2.54	0.54
1:A:9:ALA:HB3	2:B:1193:GLN:HB2	1.89	0.54
2:B:613:VAL:CG2	2:B:628:THR:HA	2.38	0.54
3:C:191:TYR:HB3	3:C:201:TRP:CD1	2.43	0.54
4:D:64:VAL:HG22	4:D:129:LEU:HD22	1.89	0.54
7:G:127:PRO:HG3	7:G:139:ILE:CD1	2.38	0.54
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.32	0.54
7:G:87:VAL:HB	7:G:103:VAL:HG11	1.90	0.54
8:H:10:PHE:O	8:H:54:SER:HA	2.08	0.54
13:T:18:DA:H1'	13:T:19:8OG:C5'	2.37	0.54
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.90	0.53
1:A:537:ARG:HD2	8:H:20:TYR:CE1	2.31	0.53
1:A:863:VAL:HG11	1:A:866:PHE:CE2	2.42	0.53
2:B:484:ASN:ND2	2:B:486:TYR:HE1	2.06	0.53
2:B:503:GLY:CA	2:B:507:LYS:HE2	2.35	0.53
2:B:510:LYS:CG	2:B:511:PRO:HD3	2.37	0.53
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.90	0.53
5:E:22:MET:HG3	5:E:187:TYR:CD1	2.43	0.53
7:G:41:LYS:HD3	7:G:42:PHE:CE1	2.42	0.53
8:H:76:THR:HG23	8:H:77:ARG:HG3	1.88	0.53
11:K:49:GLU:HA	11:K:52:ASN:HD22	1.72	0.53
1:A:547:LEU:HB3	11:K:58:PHE:CE1	2.43	0.53
1:A:211:PHE:HA	1:A:214:ILE:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:GLY:HA2	1:A:815:PHE:CD1	2.44	0.53
1:A:993:LEU:HD22	1:A:1046:LEU:HD23	1.90	0.53
2:B:67:SER:OG	2:B:68:THR:N	2.42	0.53
2:B:701:ILE:HB	2:B:739:THR:OG1	2.07	0.53
2:B:756:ILE:O	2:B:759:PRO:HD3	2.08	0.53
3:C:50:GLU:CG	12:L:64:LEU:HD22	2.39	0.53
10:J:36:LEU:HB2	10:J:47:ARG:HH12	1.72	0.53
2:B:992:ILE:HD11	11:K:66:PRO:HB2	1.90	0.53
1:A:1050:GLU:O	1:A:1053:PHE:HB3	2.08	0.53
1:A:1081:LEU:CD1	1:A:1097:GLY:HA3	2.38	0.53
1:A:1239:ARG:C	1:A:1240:CYS:SG	2.86	0.53
1:A:98:LYS:HE2	1:A:224:PHE:CZ	2.42	0.53
1:A:798:GLY:HA2	1:A:815:PHE:HD1	1.73	0.53
2:B:583:ASN:HD21	2:B:628:THR:CG2	2.21	0.53
3:C:25:VAL:HG22	3:C:228:PHE:CE1	2.43	0.53
8:H:100:THR:HG23	8:H:138:GLU:CB	2.38	0.53
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.38	0.53
1:A:1215:ARG:HG2	1:A:1215:ARG:HH11	1.73	0.53
1:A:1423:GLY:HA3	1:A:1426:GLU:HG2	1.90	0.53
1:A:923:LEU:O	1:A:927:VAL:HG23	2.09	0.53
2:B:46:GLN:HG3	2:B:47:GLN:N	2.18	0.53
2:B:642:ASP:N	2:B:649:LYS:HG3	2.24	0.53
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.89	0.53
5:E:138:ALA:HA	5:E:141:VAL:CG2	2.39	0.53
4:D:141:LEU:HD22	7:G:46:LEU:O	2.07	0.53
1:A:102:VAL:HB	1:A:211:PHE:HZ	1.71	0.53
1:A:1178:ASP:O	1:A:1179:GLU:HG3	2.09	0.53
1:A:1373:ASP:HA	1:A:1376:THR:HG22	1.90	0.53
1:A:317:LYS:O	1:A:318:SER:CB	2.56	0.53
1:A:475:THR:HG23	1:A:476:SER:N	2.24	0.53
1:A:567:LYS:CB	1:A:568:PRO:CD	2.87	0.53
2:B:1166:CYS:SG	2:B:1185:CYS:SG	3.06	0.53
3:C:133:ILE:HG21	3:C:236:GLY:HA3	1.90	0.53
2:B:1003:ALA:HA	3:C:178:PHE:O	2.09	0.53
11:K:108:GLU:O	11:K:112:GLN:HG2	2.08	0.53
12:L:39:SER:O	12:L:40:LEU:HB2	2.09	0.53
13:T:11:DA:H2"	13:T:12:DG:C8	2.43	0.53
1:A:1153:TYR:HB2	1:A:1192:LEU:HD23	1.91	0.53
1:A:125:ALA:C	1:A:127:ALA:H	2.12	0.53
1:A:1366:ARG:HG2	1:A:1366:ARG:HH11	1.73	0.53
1:A:286:HIS:O	1:A:288:ALA:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:O	1:A:322:VAL:HG13	2.08	0.53
1:A:535:THR:CG2	1:A:616:VAL:HA	2.38	0.53
1:A:756:ILE:O	1:A:759:ALA:HB3	2.09	0.53
2:B:549:THR:HG22	2:B:550:ASP:N	2.23	0.53
2:B:603:LEU:CD1	2:B:608:ASP:HB3	2.39	0.53
2:B:616:ILE:CG2	2:B:700:SER:OG	2.56	0.53
2:B:711:GLU:HB2	2:B:712:PRO:CD	2.38	0.53
8:H:89:LEU:C	8:H:91:ASP:N	2.62	0.53
9:I:85:PHE:HD2	9:I:85:PHE:N	2.04	0.53
10:J:57:ILE:O	10:J:60:PHE:HB2	2.09	0.53
1:A:1075:PRO:O	1:A:1079:MET:HG3	2.09	0.53
1:A:1201:ALA:C	1:A:1203:ASN:H	2.11	0.53
1:A:1220:PHE:CD1	1:A:1224:LEU:HD23	2.44	0.53
1:A:1291:VAL:HG13	1:A:1292:PRO:CD	2.39	0.53
1:A:289:ILE:O	1:A:292:ALA:N	2.31	0.53
2:B:216:GLU:HA	2:B:406:LEU:HD23	1.91	0.53
2:B:706:GLN:NE2	2:B:730:ARG:HD3	2.24	0.53
5:E:185:ALA:O	5:E:190:LEU:HB2	2.09	0.53
11:K:30:ALA:HB2	11:K:76:GLN:HG3	1.90	0.53
11:K:42:LEU:HD21	11:K:46:ILE:CD1	2.39	0.53
12:L:30:ILE:HG22	12:L:31:CYS:N	2.24	0.53
1:A:286:HIS:C	1:A:288:ALA:H	2.11	0.53
1:A:265:LYS:CE	1:A:302:THR:HG23	2.39	0.53
1:A:456:MET:CE	1:A:507:VAL:HG13	2.39	0.53
1:A:658:LEU:HD23	1:A:659:HIS:CE1	2.44	0.53
1:A:699:ALA:HB1	9:I:114:GLN:HE21	1.74	0.53
1:A:75:ASN:O	1:A:76:GLU:CB	2.57	0.53
2:B:616:ILE:HG23	2:B:700:SER:OG	2.09	0.53
3:C:236:GLY:O	3:C:237:SER:C	2.46	0.53
4:D:63:LEU:O	4:D:129:LEU:HD11	2.08	0.53
5:E:182:ASP:HB3	5:E:185:ALA:HB2	1.91	0.53
5:E:83:CYS:C	5:E:85:GLU:H	2.11	0.53
8:H:40:LEU:HD22	8:H:123:MET:CE	2.39	0.53
9:I:55:THR:HG23	9:I:86:PHE:HZ	1.73	0.53
10:J:20:SER:O	10:J:24:LEU:HG	2.08	0.53
1:A:150:THR:HG23	1:A:165:GLY:O	2.09	0.53
1:A:219:PHE:CE1	1:A:230:ARG:HD3	2.44	0.53
1:A:326:ARG:HG3	1:A:327:ALA:N	2.24	0.53
1:A:42:ASP:OD2	1:A:45:GLN:HA	2.09	0.53
1:A:537:ARG:HH22	8:H:122:LEU:CD1	2.22	0.53
1:A:57:ARG:O	1:A:58:LEU:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:999:MET:HG2	2:B:1007:VAL:HG22	1.91	0.53
2:B:203:PHE:N	2:B:203:PHE:CD1	2.77	0.53
2:B:29:ASP:OD1	2:B:658:ILE:HD13	2.09	0.53
2:B:687:GLU:HB3	2:B:689:LEU:HG	1.91	0.53
4:D:70:PHE:O	4:D:74:GLN:NE2	2.42	0.53
5:E:176:PRO:O	5:E:212:ARG:HA	2.09	0.53
1:A:1264:GLU:HG3	1:A:1265:ASN:N	2.24	0.53
1:A:1449:SER:HB2	1:A:1453:TYR:CE1	2.44	0.53
1:A:266:LEU:HD21	1:A:303:TYR:CZ	2.44	0.53
1:A:503:GLN:C	1:A:504:LEU:HD12	2.29	0.53
1:A:600:PRO:CG	1:A:601:LYS:H	2.13	0.53
1:A:777:PHE:CD1	1:A:781:ASP:HA	2.44	0.53
2:B:221:ASN:N	2:B:241:ARG:O	2.41	0.53
2:B:284:ILE:HG23	2:B:324:ILE:HD13	1.91	0.53
3:C:182:PRO:HD2	3:C:210:GLU:OE1	2.09	0.53
4:D:126:ILE:HD13	4:D:145:MET:CE	2.39	0.53
5:E:110:PHE:HE2	5:E:112:TYR:HB3	1.73	0.53
7:G:13:LEU:CD2	7:G:14:HIS:N	2.73	0.53
3:C:66:ARG:NH2	10:J:3:VAL:O	2.42	0.53
2:B:190:TYR:CE2	10:J:62:ARG:HD3	2.44	0.53
13:T:22:DC:H2'	13:T:23:BRU:H6	1.90	0.53
1:A:108:MET:CB	1:A:210:ILE:HD13	2.26	0.52
1:A:88:LYS:HE3	1:A:280:GLU:OE2	2.09	0.52
1:A:41:MET:N	1:A:41:MET:HE3	2.24	0.52
1:A:569:LYS:O	1:A:571:LEU:HD13	2.09	0.52
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.44	0.52
2:B:863:GLU:OE2	2:B:873:THR:HA	2.09	0.52
3:C:89:GLU:O	3:C:90:ASP:CB	2.57	0.52
4:D:118:THR:CB	4:D:121:LYS:HB2	2.38	0.52
2:B:1165:ILE:HD13	4:D:17:LYS:HD3	1.90	0.52
5:E:91:LYS:C	5:E:93:MET:H	2.13	0.52
1:A:350:ARG:HG3	1:A:350:ARG:HH11	1.73	0.52
1:A:452:LYS:HE3	2:B:1141:HIS:CE1	2.44	0.52
1:A:57:ARG:HH11	1:A:57:ARG:HG2	1.74	0.52
1:A:664:THR:HG22	1:A:665:GLY:N	2.24	0.52
2:B:1084:GLN:HE21	2:B:1084:GLN:H	1.57	0.52
2:B:1150:ARG:NH1	2:B:1150:ARG:CG	2.67	0.52
2:B:1167:GLY:HA3	2:B:1216:LEU:H	1.74	0.52
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.90	0.52
2:B:291:ILE:HG22	2:B:291:ILE:O	2.08	0.52
2:B:582:VAL:HB	2:B:587:HIS:HD2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:990:ILE:HG22	2:B:991:GLY:N	2.24	0.52
3:C:152:GLU:HG2	3:C:153:LEU:H	1.72	0.52
5:E:22:MET:O	5:E:26:ARG:HB2	2.09	0.52
9:I:111:THR:CG2	9:I:112:SER:N	2.71	0.52
1:A:164:ARG:HG3	1:A:165:GLY:N	2.24	0.52
1:A:279:LEU:O	1:A:289:ILE:HD11	2.09	0.52
1:A:315:LEU:HD22	1:A:319:GLY:O	2.08	0.52
1:A:689:LYS:HE2	1:A:721:PHE:CZ	2.45	0.52
1:A:904:THR:O	1:A:904:THR:HG22	2.09	0.52
2:B:227:LYS:HB2	2:B:395:GLN:OE1	2.08	0.52
2:B:549:THR:HG22	2:B:550:ASP:H	1.75	0.52
2:B:601:ARG:C	2:B:603:LEU:H	2.11	0.52
2:B:65:GLU:HG3	2:B:66:ASP:H	1.74	0.52
2:B:723:VAL:CG1	2:B:724:ASP:H	2.11	0.52
3:C:75:MET:O	3:C:246:ARG:NH2	2.42	0.52
6:F:119:ARG:HG3	6:F:119:ARG:NH1	2.24	0.52
7:G:140:LYS:O	7:G:141:SER:C	2.47	0.52
13:T:10:DA:C2	13:T:11:DA:C4	2.97	0.52
1:A:390:GLN:O	1:A:394:ASN:N	2.42	0.52
1:A:897:TYR:CD1	1:A:897:TYR:N	2.77	0.52
1:A:16:GLU:HG3	2:B:1220:ARG:HA	1.91	0.52
2:B:188:ASP:C	2:B:192:LEU:HD12	2.30	0.52
2:B:546:SER:HA	2:B:612:GLU:OE2	2.10	0.52
2:B:559:SER:CA	2:B:563:MET:HB3	2.29	0.52
2:B:871:THR:HG22	2:B:872:GLU:N	2.24	0.52
3:C:167:HIS:ND1	3:C:169:LYS:HG2	2.25	0.52
4:D:52:LEU:HA	4:D:148:LEU:HD21	1.91	0.52
5:E:110:PHE:CE2	5:E:112:TYR:HB3	2.44	0.52
5:E:207:ARG:HH11	5:E:207:ARG:HB3	1.75	0.52
6:F:116:ASP:O	6:F:120:ILE:HG13	2.09	0.52
7:G:45:ILE:HD13	7:G:78:VAL:CG1	2.40	0.52
8:H:44:VAL:CG1	8:H:48:PRO:HA	2.40	0.52
10:J:24:LEU:HD12	10:J:39:LEU:HD11	1.90	0.52
12:L:41:SER:O	12:L:44:ASP:HB2	2.10	0.52
1:A:262:LEU:HD21	1:A:303:TYR:HE1	1.75	0.52
1:A:401:GLY:C	1:A:435:HIS:CD2	2.83	0.52
1:A:591:PHE:HA	1:A:595:THR:CG2	2.37	0.52
1:A:655:PHE:O	1:A:658:LEU:HB3	2.09	0.52
1:A:683:ILE:HD13	1:A:801:GLU:CG	2.38	0.52
1:A:884:ASP:HB3	1:A:896:ARG:HH12	1.74	0.52
1:A:899:VAL:HG13	1:A:908:LEU:CD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:744:HIS:HD2	2:B:746:SER:OG	1.93	0.52
2:B:542:MET:SD	2:B:747:MET:HE2	2.49	0.52
2:B:847:ASP:C	2:B:849:GLY:N	2.63	0.52
3:C:147:LEU:HD12	3:C:151:GLN:O	2.10	0.52
4:D:154:PHE:CD1	4:D:154:PHE:N	2.78	0.52
4:D:41:GLN:HB2	4:D:43:GLU:HG3	1.92	0.52
5:E:153:HIS:O	5:E:154:ILE:HG13	2.09	0.52
5:E:55:ARG:O	5:E:57:MET:N	2.43	0.52
6:F:127:GLU:O	6:F:129:LYS:HG3	2.09	0.52
7:G:99:PHE:HZ	7:G:163:ILE:HD13	1.74	0.52
9:I:82:GLU:HB3	9:I:104:LEU:CD1	2.40	0.52
1:A:1001:ARG:O	1:A:1002:GLY:O	2.28	0.52
1:A:157:ASP:C	1:A:159:THR:H	2.12	0.52
1:A:172:PRO:HD3	1:A:185:TRP:NE1	2.24	0.52
1:A:567:LYS:HB3	1:A:568:PRO:CD	2.37	0.52
1:A:944:ARG:NE	1:A:1298:TYR:HE1	2.07	0.52
3:C:33:LEU:O	3:C:34:ARG:C	2.48	0.52
4:D:54:GLU:O	4:D:58:VAL:HG23	2.10	0.52
3:C:235:VAL:HG12	10:J:13:VAL:HG23	1.91	0.52
1:A:1036:ARG:HG2	1:A:1036:ARG:NH1	2.25	0.52
1:A:108:MET:O	1:A:109:HIS:HB2	2.09	0.52
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.29	0.52
1:A:188:ASP:CB	1:A:191:THR:HB	2.33	0.52
1:A:196:GLU:CB	1:A:197:PRO:HD2	2.36	0.52
1:A:317:LYS:O	1:A:318:SER:HB3	2.09	0.52
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.43	0.52
2:B:1095:LEU:C	2:B:1096:ARG:O	2.46	0.52
2:B:196:PRO:HG2	2:B:197:PHE:H	1.74	0.52
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.44	0.52
3:C:152:GLU:HG2	3:C:153:LEU:N	2.24	0.52
4:D:56:ARG:NH2	4:D:155:ARG:HA	2.25	0.52
4:D:51:ASN:O	4:D:52:LEU:C	2.48	0.52
8:H:76:THR:O	8:H:77:ARG:HB2	2.09	0.52
9:I:69:PRO:HB2	9:I:85:PHE:CE2	2.45	0.52
1:A:1127:ASP:HB3	1:A:1130:GLN:CB	2.39	0.52
1:A:1156:PRO:HA	1:A:1190:PRO:HB3	1.92	0.52
1:A:1289:ARG:HD2	1:A:1303:GLU:OE2	2.09	0.52
1:A:1118:VAL:O	1:A:1305:VAL:HG13	2.09	0.52
1:A:15:LYS:HG3	2:B:1219:ASP:HA	1.92	0.52
1:A:350:ARG:NH1	1:A:350:ARG:HG3	2.24	0.52
1:A:475:THR:CG2	1:A:476:SER:N	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:ILE:O	1:A:973:ILE:HG22	2.09	0.52
2:B:613:VAL:HG13	2:B:627:PHE:C	2.30	0.52
3:C:125:MET:HG3	3:C:127:ARG:NH2	2.25	0.52
5:E:31:THR:HG23	5:E:34:GLU:CB	2.38	0.52
1:A:1115:SER:O	1:A:1116:LEU:HB2	2.10	0.52
1:A:531:ILE:HD11	1:A:578:LEU:HD11	1.91	0.52
1:A:645:LEU:HG	1:A:649:ILE:HD11	1.91	0.52
1:A:896:ARG:HB3	1:A:897:TYR:CD1	2.45	0.52
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.74	0.52
1:A:936:LEU:O	1:A:939:ASP:HB2	2.10	0.52
1:A:18:GLN:HB2	2:B:1215:ARG:HB2	1.91	0.52
2:B:205:ILE:N	2:B:205:ILE:HD12	2.25	0.52
2:B:806:THR:HB	2:B:809:MET:HG3	1.92	0.52
6:F:130:ILE:HG22	6:F:132:LEU:HG	1.91	0.52
9:I:26:LEU:HD23	9:I:37:GLU:CA	2.36	0.52
1:A:320:ARG:NH2	15:P:3:U:O2'	2.42	0.52
1:A:1152:ILE:HG23	1:A:1193:LEU:HD13	1.92	0.52
1:A:396:PRO:HB3	1:A:402:ALA:O	2.09	0.52
1:A:399:HIS:CB	1:A:400:PRO:CD	2.88	0.52
1:A:629:LEU:HD11	1:A:645:LEU:HD21	1.92	0.52
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.92	0.52
1:A:858:ASN:ND2	1:A:860:LEU:H	2.08	0.52
2:B:1084:GLN:HE21	2:B:1084:GLN:N	2.07	0.52
1:A:2:VAL:HG11	2:B:1157:ALA:C	2.31	0.52
2:B:254:LEU:CD1	2:B:273:LEU:HD23	2.40	0.52
2:B:620:ARG:NH2	9:I:89:GLN:NE2	2.57	0.52
2:B:750:GLY:O	2:B:751:VAL:C	2.47	0.52
1:A:537:ARG:HH22	8:H:122:LEU:HG	1.74	0.52
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.92	0.52
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.84	0.52
12:L:28:LYS:HB2	12:L:39:SER:HB2	1.91	0.52
1:A:1162:VAL:HG11	9:I:41:PRO:HG3	1.91	0.51
1:A:1173:HIS:ND1	1:A:1173:HIS:O	2.43	0.51
2:B:113:TYR:HB3	2:B:114:PRO:HD2	1.91	0.51
2:B:192:LEU:O	2:B:193:LYS:HB2	2.09	0.51
2:B:269:ILE:CG2	2:B:282:ILE:HD13	2.40	0.51
2:B:294:ASP:HB2	9:I:12:ASN:HA	1.92	0.51
2:B:521:LEU:HD13	2:B:633:VAL:CG1	2.40	0.51
2:B:770:GLN:HG2	2:B:983:ARG:O	2.09	0.51
4:D:53:SER:H	4:D:148:LEU:HD22	1.71	0.51
9:I:62:ILE:HG12	9:I:62:ILE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1154:TYR:HD1	1:A:1191:TRP:CZ3	2.28	0.51
1:A:200:ARG:HG3	1:A:201:VAL:N	2.25	0.51
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.09	0.51
1:A:560:ILE:HD12	8:H:79:TRP:HB3	1.92	0.51
1:A:685:GLU:OE2	1:A:686:ALA:HB2	2.11	0.51
2:B:102:VAL:HB	2:B:110:HIS:HB3	1.92	0.51
2:B:1162:ILE:HD11	2:B:1194:ILE:CD1	2.41	0.51
2:B:216:GLU:HB3	2:B:500:THR:CG2	2.37	0.51
2:B:314:LEU:O	2:B:317:CYS:HB3	2.11	0.51
2:B:327:ARG:HG2	2:B:327:ARG:O	2.10	0.51
2:B:360:PHE:O	2:B:361:LEU:C	2.49	0.51
2:B:68:THR:OG1	2:B:91:SER:CB	2.58	0.51
2:B:806:THR:HG22	2:B:807:ARG:N	2.24	0.51
3:C:176:ILE:HG22	3:C:177:GLU:H	1.74	0.51
3:C:18:VAL:O	3:C:20:PHE:HD2	1.93	0.51
5:E:124:VAL:CG1	5:E:132:ILE:HG13	2.39	0.51
7:G:137:ILE:HG21	7:G:143:ILE:HD11	1.93	0.51
1:A:1151:GLU:OE2	9:I:45:ARG:HD2	2.10	0.51
1:A:700:ASN:HB2	9:I:98:VAL:HG21	1.92	0.51
1:A:10:PRO:HG2	2:B:1191:ILE:O	2.09	0.51
1:A:1163:ILE:HG22	1:A:1165:GLU:HG2	1.91	0.51
1:A:12:ARG:CB	2:B:1218:THR:HG22	2.38	0.51
1:A:630:ILE:HG23	1:A:631:HIS:H	1.74	0.51
1:A:672:ASP:OD2	1:A:674:PRO:HG2	2.10	0.51
1:A:942:PHE:HZ	5:E:207:ARG:HG3	1.75	0.51
2:B:176:SER:O	2:B:182:SER:HB3	2.10	0.51
2:B:100:PRO:HD2	2:B:180:TYR:HE1	1.73	0.51
2:B:38:PHE:CD1	2:B:811:TYR:HD2	2.29	0.51
2:B:558:LEU:O	2:B:560:GLU:N	2.38	0.51
2:B:547:VAL:HG12	2:B:612:GLU:OE2	2.10	0.51
2:B:616:ILE:HD12	2:B:616:ILE:N	2.25	0.51
4:D:63:LEU:HD12	4:D:129:LEU:HG	1.92	0.51
4:D:150:ASN:HB3	7:G:142:ARG:HH22	1.75	0.51
4:D:51:ASN:O	4:D:52:LEU:O	2.27	0.51
7:G:143:ILE:CG2	7:G:144:ARG:H	2.23	0.51
7:G:88:ASP:OD2	7:G:88:ASP:N	2.42	0.51
11:K:12:LEU:H	11:K:12:LEU:CD1	2.18	0.51
12:L:68:GLU:OE1	12:L:68:GLU:N	2.27	0.51
1:A:332:LYS:HB2	1:A:337:ARG:HH11	1.75	0.51
1:A:72:GLU:O	1:A:73:GLY:O	2.29	0.51
1:A:830:LYS:HE2	1:A:1081:LEU:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:LYS:HD3	2:B:482:VAL:HG12	1.93	0.51
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.92	0.51
2:B:44:VAL:HG23	2:B:48:LEU:HD11	1.90	0.51
2:B:46:GLN:HE22	2:B:496:ARG:CB	2.24	0.51
1:A:816:HIS:HE2	2:B:764:SER:H	1.58	0.51
3:C:123:ASN:C	3:C:125:MET:H	2.12	0.51
3:C:146:LYS:C	3:C:147:LEU:HD23	2.30	0.51
2:B:1067:ARG:NH2	3:C:194:GLU:OE2	2.43	0.51
5:E:181:ALA:O	5:E:182:ASP:C	2.49	0.51
8:H:11:GLN:HA	8:H:53:ASP:O	2.09	0.51
8:H:129:TYR:HA	8:H:131:ASN:HD21	1.75	0.51
11:K:10:PHE:CD2	11:K:10:PHE:N	2.78	0.51
3:C:166:GLU:C	11:K:6:ARG:NH1	2.64	0.51
1:A:1039:LYS:HE3	1:A:1043:ASP:OD2	2.10	0.51
1:A:1191:TRP:HA	1:A:1191:TRP:CE3	2.44	0.51
1:A:889:SER:HB3	1:A:1297:GLU:CG	2.41	0.51
1:A:35:ILE:O	1:A:35:ILE:HG22	2.11	0.51
1:A:443:LEU:HD23	1:A:501:LEU:HD21	1.90	0.51
1:A:592:ASP:N	1:A:595:THR:OG1	2.44	0.51
1:A:844:ALA:HB2	1:A:1389:PHE:CE2	2.46	0.51
2:B:293:PRO:O	2:B:297:ILE:HG13	2.11	0.51
2:B:283:VAL:CG2	2:B:317:CYS:O	2.59	0.51
2:B:376:PHE:CZ	2:B:569:TYR:HB3	2.46	0.51
2:B:214:ALA:HB3	2:B:497:ARG:O	2.10	0.51
2:B:547:VAL:N	2:B:612:GLU:OE2	2.41	0.51
2:B:648:HIS:CD2	2:B:649:LYS:H	2.28	0.51
4:D:187:THR:HG22	4:D:189:ASP:H	1.75	0.51
4:D:7:THR:HG23	4:D:9:GLN:H	1.75	0.51
5:E:52:ARG:CG	5:E:52:ARG:HH11	2.23	0.51
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.41	0.51
10:J:1:MET:N	10:J:57:ILE:H	2.07	0.51
10:J:7:CYS:SG	10:J:49:MET:HE3	2.50	0.51
1:A:1166:ASP:O	1:A:1168:GLU:N	2.43	0.51
1:A:108:MET:HA	1:A:210:ILE:HG21	1.91	0.51
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.46	0.51
2:B:1081:LEU:O	2:B:1083:ALA:N	2.44	0.51
2:B:244:LEU:HD21	2:B:366:GLN:HE21	1.76	0.51
2:B:65:GLU:OE1	2:B:418:LYS:HE3	2.10	0.51
3:C:260:LEU:O	3:C:264:GLN:HG3	2.10	0.51
4:D:207:LEU:O	4:D:211:LEU:HB2	2.11	0.51
5:E:67:GLU:O	5:E:70:SER:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:118:PHE:C	8:H:120:GLY:H	2.14	0.51
8:H:4:THR:HA	8:H:60:ALA:CB	2.40	0.51
9:I:4:PHE:CE1	9:I:6:PHE:HE2	2.27	0.51
1:A:1313:LEU:C	1:A:1315:GLU:H	2.14	0.51
1:A:230:ARG:HG3	1:A:233:TRP:CZ3	2.46	0.51
1:A:265:LYS:HG3	1:A:265:LYS:O	2.11	0.51
2:B:128:LEU:N	2:B:128:LEU:HD12	2.25	0.51
2:B:288:ALA:O	2:B:331:LEU:HD11	2.11	0.51
2:B:875:GLU:HG3	2:B:877:PRO:HD3	1.92	0.51
3:C:77:ILE:N	3:C:129:ILE:HD11	2.26	0.51
4:D:123:LEU:HG	4:D:149:THR:HG21	1.91	0.51
11:K:68:PHE:CB	11:K:70:ARG:HH11	2.21	0.51
1:A:384:ASN:O	1:A:387:ARG:N	2.43	0.51
1:A:556:TRP:CE3	1:A:558:GLY:HA2	2.46	0.51
1:A:899:VAL:CG1	1:A:908:LEU:HD21	2.40	0.51
2:B:1001:PHE:CE2	3:C:34:ARG:NE	2.79	0.51
2:B:1161:HIS:NE2	2:B:1175:LEU:HD21	2.25	0.51
2:B:798:TYR:CZ	3:C:62:PHE:HE2	2.28	0.51
2:B:837:ASP:O	2:B:988:GLY:HA2	2.10	0.51
3:C:33:LEU:HG	3:C:37:MET:HE1	1.91	0.51
3:C:3:GLU:HG3	11:K:104:ASN:ND2	2.26	0.51
8:H:31:THR:O	8:H:31:THR:HG22	2.10	0.51
9:I:101:PHE:N	9:I:101:PHE:CD1	2.78	0.51
9:I:86:PHE:CE1	9:I:100:PHE:HB2	2.46	0.51
1:A:146:MET:HB3	1:A:171:GLN:O	2.11	0.51
1:A:666:ILE:HG23	2:B:1026:LEU:CB	2.41	0.51
3:C:215:GLU:O	3:C:216:GLY:C	2.49	0.51
4:D:202:ILE:HD11	4:D:206:GLU:HB3	1.93	0.51
7:G:1:MET:HE1	7:G:80:LYS:H	1.74	0.51
11:K:10:PHE:HA	11:K:37:LYS:HB3	1.92	0.51
1:A:1167:GLU:O	1:A:1170:ILE:HG13	2.10	0.51
1:A:1215:ARG:HG2	1:A:1215:ARG:NH1	2.25	0.51
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.93	0.51
1:A:180:LYS:HZ2	1:A:294:SER:HB3	1.76	0.51
1:A:817:ALA:O	1:A:820:GLY:N	2.44	0.51
2:B:1106:ARG:HD3	2:B:1127:GLY:CA	2.41	0.51
2:B:326:ASP:O	2:B:328:GLU:N	2.43	0.51
5:E:117:THR:HB	5:E:120:ALA:HB2	1.93	0.51
9:I:78:CYS:SG	9:I:105:SER:HB2	2.51	0.51
1:A:440:ASP:O	1:A:442:VAL:HG22	2.11	0.50
1:A:699:ALA:CB	9:I:114:GLN:HE21	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:VAL:O	1:A:720:ARG:C	2.48	0.50
2:B:613:VAL:HG13	2:B:628:THR:HA	1.93	0.50
2:B:63:ILE:HD12	2:B:421:PHE:CE2	2.46	0.50
2:B:944:THR:HG21	2:B:1122:ARG:HH21	1.68	0.50
3:C:107:SER:C	3:C:109:SER:N	2.65	0.50
4:D:53:SER:CB	4:D:152:SER:HB2	2.41	0.50
5:E:149:LEU:HD23	5:E:149:LEU:N	2.26	0.50
8:H:101:ALA:HA	8:H:116:TYR:HA	1.92	0.50
8:H:84:ALA:HA	8:H:87:ARG:CG	2.41	0.50
8:H:89:LEU:CB	8:H:91:ASP:OD1	2.59	0.50
9:I:13:MET:HE3	9:I:14:LEU:H	1.75	0.50
12:L:24:THR:O	12:L:25:ALA:HB3	2.11	0.50
1:A:1273:LEU:N	1:A:1273:LEU:HD12	2.25	0.50
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.92	0.50
1:A:149:GLU:HB2	1:A:164:ARG:HH21	1.76	0.50
1:A:170:THR:HG22	1:A:171:GLN:N	2.25	0.50
1:A:35:ILE:CD1	1:A:241:VAL:HG21	2.41	0.50
1:A:472:LEU:O	1:A:475:THR:CB	2.57	0.50
2:B:1034:VAL:C	2:B:1036:ALA:H	2.13	0.50
2:B:185:THR:O	2:B:186:GLU:C	2.49	0.50
2:B:778:MET:CE	2:B:853:SER:HB3	2.41	0.50
5:E:128:PRO:HA	5:E:129:PRO:C	2.31	0.50
6:F:70:LYS:O	6:F:72:LYS:N	2.35	0.50
15:P:4:C:H2'	15:P:5:C:C6	2.46	0.50
1:A:1118:VAL:HG12	1:A:1327:ILE:HG13	1.92	0.50
1:A:149:GLU:HB2	1:A:164:ARG:NH2	2.27	0.50
1:A:225:ASN:ND2	1:A:228:PHE:N	2.53	0.50
1:A:698:GLN:NE2	9:I:99:LEU:HD11	2.26	0.50
1:A:803:SER:OG	1:A:806:ARG:HG3	2.12	0.50
2:B:542:MET:HG2	2:B:747:MET:HE3	1.94	0.50
2:B:597:MET:HE3	2:B:600:LEU:HD12	1.93	0.50
2:B:60:GLN:NE2	2:B:94:LYS:HA	2.26	0.50
3:C:100:THR:CG2	3:C:102:GLN:NE2	2.75	0.50
4:D:185:CYS:O	4:D:211:LEU:HD22	2.10	0.50
8:H:39:THR:O	8:H:123:MET:HG3	2.11	0.50
1:A:560:ILE:CG1	8:H:79:TRP:H	2.24	0.50
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.45	0.50
10:J:1:MET:H1	10:J:56:LEU:HB2	1.75	0.50
1:A:1070:GLN:O	1:A:1074:GLU:HB2	2.11	0.50
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.11	0.50
1:A:269:ILE:CG1	1:A:299:HIS:HB3	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:GLY:C	1:A:312:PRO:HD2	2.31	0.50
1:A:919:ILE:HG21	1:A:983:ILE:CD1	2.42	0.50
2:B:827:ILE:O	2:B:1085:ILE:HG23	2.11	0.50
2:B:340:ALA:CB	2:B:343:ILE:HG12	2.24	0.50
2:B:703:ILE:HG23	2:B:741:CYS:HA	1.92	0.50
2:B:880:THR:CB	2:B:934:LYS:HD3	2.38	0.50
4:D:19:GLU:O	4:D:20:GLU:C	2.50	0.50
4:D:24:ALA:O	4:D:26:THR:N	2.44	0.50
8:H:81:PRO:HB2	8:H:82:PRO:HD3	1.91	0.50
9:I:111:THR:HG21	9:I:113:ASP:HB2	1.93	0.50
1:A:1156:PRO:HA	1:A:1190:PRO:CB	2.42	0.50
1:A:326:ARG:HH22	1:A:1407:GLU:HG2	1.76	0.50
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.92	0.50
2:B:313:MET:CE	2:B:390:LEU:HD11	2.42	0.50
2:B:358:LYS:HA	2:B:366:GLN:HB3	1.92	0.50
2:B:521:LEU:HD13	2:B:633:VAL:CB	2.42	0.50
1:A:802:ASN:ND2	2:B:728:ARG:HB2	2.27	0.50
4:D:67:ARG:CA	4:D:133:THR:HG21	2.41	0.50
4:D:191:ALA:CB	4:D:207:LEU:HD21	2.42	0.50
4:D:206:GLU:O	4:D:210:ILE:HG13	2.11	0.50
4:D:185:CYS:HB2	4:D:211:LEU:HD21	1.92	0.50
4:D:26:THR:O	4:D:26:THR:HG22	2.12	0.50
6:F:73:ALA:HB1	6:F:143:PHE:H	1.76	0.50
7:G:4:ILE:HA	7:G:76:ALA:O	2.12	0.50
8:H:63:LEU:HD13	8:H:64:ASN:H	1.77	0.50
11:K:31:VAL:CG1	11:K:32:VAL:H	2.18	0.50
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.93	0.50
12:L:47:ARG:NH2	12:L:54:ARG:HE	2.09	0.50
1:A:404:TYR:HB2	1:A:433:GLU:HB2	1.94	0.50
1:A:734:GLU:C	1:A:736:ASN:H	2.14	0.50
1:A:775:ILE:HD12	1:A:818:MET:SD	2.52	0.50
1:A:863:VAL:HG11	1:A:866:PHE:CD2	2.46	0.50
1:A:886:ILE:CG2	1:A:887:GLY:N	2.74	0.50
2:B:179:CYS:SG	2:B:181:LEU:HB2	2.51	0.50
2:B:461:LEU:CD1	2:B:461:LEU:H	2.24	0.50
2:B:579:ARG:CA	2:B:589:VAL:HG22	2.40	0.50
2:B:847:ASP:HB3	3:C:167:HIS:NE2	2.26	0.50
11:K:53:ASP:HB3	11:K:56:VAL:CG2	2.40	0.50
1:A:1011:GLN:NE2	1:A:1015:VAL:CG2	2.75	0.50
1:A:102:VAL:HG11	1:A:211:PHE:CE2	2.47	0.50
1:A:896:ARG:NH2	1:A:1030:ARG:HH21	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1067:LEU:O	1:A:1068:ALA:C	2.48	0.50
1:A:113:LEU:O	1:A:114:LEU:HD23	2.12	0.50
1:A:113:LEU:C	1:A:114:LEU:HD23	2.32	0.50
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.11	0.50
1:A:1209:MET:CE	1:A:1236:LEU:HB3	2.42	0.50
1:A:42:ASP:C	1:A:44:THR:N	2.65	0.50
1:A:567:LYS:CD	1:A:568:PRO:HD3	2.41	0.50
1:A:767:GLN:HA	1:A:799:PHE:HA	1.93	0.50
1:A:343:LYS:HD3	2:B:1155:SER:OG	2.11	0.50
2:B:842:ASN:ND2	2:B:845:SER:H	2.10	0.50
5:E:124:VAL:HG13	5:E:132:ILE:CB	2.42	0.50
5:E:153:HIS:HB3	5:E:196:VAL:HG11	1.94	0.50
6:F:117:PRO:C	6:F:119:ARG:H	2.15	0.50
1:A:1093:LYS:O	1:A:1094:VAL:HG13	2.12	0.50
1:A:95:PHE:CD1	1:A:234:MET:HG2	2.47	0.50
1:A:41:MET:CB	1:A:50:ILE:H	2.25	0.50
1:A:551:TYR:CD2	11:K:62:LYS:HD3	2.47	0.50
1:A:555:ASP:O	1:A:556:TRP:C	2.50	0.50
1:A:568:PRO:HD2	1:A:569:LYS:H	1.76	0.50
1:A:590:ARG:HG3	1:A:590:ARG:HH11	1.77	0.50
1:A:598:LEU:O	1:A:599:SER:C	2.50	0.50
1:A:771:GLU:O	1:A:773:LYS:HG3	2.11	0.50
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.93	0.50
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.51	0.50
2:B:370:PHE:HE2	2:B:373:ARG:HH11	1.57	0.50
2:B:641:GLU:C	2:B:643:ASP:H	2.14	0.50
2:B:67:SER:O	2:B:68:THR:O	2.30	0.50
4:D:202:ILE:HG23	4:D:207:LEU:HB2	1.93	0.50
5:E:94:LYS:HG3	5:E:98:ILE:CD1	2.41	0.50
6:F:74:ILE:HD12	6:F:144:GLU:HG3	1.93	0.50
7:G:18:PHE:HA	7:G:22:MET:CE	2.42	0.50
8:H:83:GLN:C	8:H:85:GLY:H	2.15	0.50
1:A:374:LEU:O	1:A:436:ILE:HG12	2.11	0.50
1:A:590:ARG:HB2	1:A:605:MET:HB3	1.94	0.50
2:B:96:TYR:N	2:B:129:PHE:O	2.43	0.50
2:B:357:GLN:O	2:B:366:GLN:HA	2.12	0.50
3:C:182:PRO:HG3	3:C:206:ASN:O	2.12	0.50
4:D:168:LYS:HG3	4:D:177:VAL:CG1	2.35	0.50
5:E:45:LYS:HB3	5:E:46:TYR:CD1	2.47	0.50
2:B:1189:ILE:HD11	7:G:39:THR:HG23	1.93	0.50
8:H:100:THR:O	8:H:117:SER:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:16:ASP:OD1	10:J:17:LYS:HD2	2.11	0.50
11:K:49:GLU:OE2	11:K:97:LYS:HE3	2.12	0.50
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.27	0.49
1:A:335:ARG:HD3	2:B:1202:LEU:HD23	1.93	0.49
1:A:63:ARG:HG3	1:A:63:ARG:O	2.12	0.49
1:A:700:ASN:ND2	9:I:115:LYS:HD2	2.27	0.49
1:A:781:ASP:O	1:A:790:ASP:N	2.46	0.49
2:B:284:ILE:HG12	2:B:324:ILE:HD12	1.94	0.49
2:B:526:GLU:O	2:B:526:GLU:HG2	2.11	0.49
2:B:563:MET:HE1	2:B:580:VAL:HB	1.94	0.49
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.47	0.49
3:C:8:VAL:HG12	3:C:9:LYS:N	2.25	0.49
5:E:134:THR:C	5:E:135:PHE:HD1	2.15	0.49
8:H:100:THR:HG22	8:H:101:ALA:H	1.76	0.49
8:H:102:TYR:CE2	8:H:115:TYR:HB3	2.47	0.49
8:H:15:VAL:HG13	8:H:26:ILE:CG1	2.37	0.49
1:A:280:GLU:C	1:A:282:ASN:N	2.65	0.49
1:A:393:ARG:CB	1:A:393:ARG:HH11	2.26	0.49
1:A:32:VAL:O	1:A:57:ARG:CD	2.61	0.49
1:A:596:THR:O	1:A:597:LEU:HB2	2.12	0.49
1:A:676:MET:O	1:A:679:ILE:HB	2.11	0.49
2:B:165:VAL:HG12	2:B:166:PHE:N	2.27	0.49
2:B:360:PHE:HD2	2:B:374:LYS:HD3	1.77	0.49
2:B:604:ARG:HG3	2:B:611:PRO:HA	1.93	0.49
2:B:661:LEU:HG	2:B:679:TYR:CD2	2.47	0.49
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.27	0.49
2:B:1084:GLN:OE1	3:C:189:THR:CG2	2.60	0.49
7:G:74:TYR:H	7:G:74:TYR:HD2	1.59	0.49
9:I:50:THR:HG22	9:I:52:ILE:H	1.77	0.49
1:A:1265:ASN:O	1:A:1266:THR:C	2.51	0.49
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.75	0.49
1:A:865:GLN:NE2	1:A:1370:LEU:HA	2.28	0.49
1:A:208:LEU:HD23	1:A:209:ASN:N	2.27	0.49
1:A:243:PRO:CB	1:A:244:PRO:HD2	2.40	0.49
1:A:427:GLN:O	1:A:430:TRP:HB2	2.12	0.49
1:A:492:PRO:O	1:A:493:GLN:NE2	2.45	0.49
1:A:523:ILE:HD11	1:A:649:ILE:HB	1.93	0.49
1:A:546:VAL:HG13	1:A:577:ILE:HG21	1.93	0.49
1:A:590:ARG:HD3	1:A:592:ASP:OD2	2.12	0.49
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.94	0.49
1:A:944:ARG:CZ	1:A:1298:TYR:HE1	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1001:PHE:CD2	3:C:34:ARG:NH2	2.80	0.49
2:B:1002:THR:CG2	2:B:1006:ILE:CG1	2.80	0.49
2:B:1077:THR:HG22	11:K:44:ASN:ND2	2.26	0.49
2:B:244:LEU:HD11	2:B:366:GLN:NE2	2.21	0.49
2:B:313:MET:HE2	2:B:390:LEU:HD11	1.93	0.49
2:B:377:PHE:O	2:B:380:TYR:N	2.45	0.49
2:B:213:ILE:HD11	2:B:497:ARG:H	1.77	0.49
2:B:707:PRO:HG2	2:B:708:GLU:H	1.77	0.49
2:B:857:ARG:NH2	2:B:942:ARG:NH2	2.60	0.49
3:C:258:ILE:O	3:C:262:LEU:HG	2.11	0.49
5:E:186:LEU:N	5:E:186:LEU:HD23	2.27	0.49
7:G:23:LYS:HG3	7:G:56:ILE:HD12	1.95	0.49
4:D:29:LEU:HD22	7:G:82:PHE:CE2	2.47	0.49
1:A:100:LYS:O	1:A:104:GLU:HG3	2.13	0.49
1:A:1161:THR:C	1:A:1163:ILE:N	2.65	0.49
1:A:1443:VAL:CG1	6:F:132:LEU:HD13	2.42	0.49
1:A:331:GLY:O	1:A:332:LYS:O	2.31	0.49
1:A:464:PRO:HG2	1:A:465:TYR:HD1	1.77	0.49
1:A:524:VAL:HG12	1:A:525:GLN:CG	2.41	0.49
1:A:666:ILE:HD11	2:B:1086:PHE:HE1	1.77	0.49
1:A:683:ILE:HG21	1:A:801:GLU:CD	2.32	0.49
1:A:971:PHE:O	1:A:973:ILE:N	2.45	0.49
2:B:1020:ARG:HG3	2:B:1020:ARG:HH11	1.76	0.49
2:B:766:ARG:HG3	2:B:1022:THR:CG2	2.42	0.49
2:B:455:SER:O	2:B:456:GLY:C	2.49	0.49
2:B:604:ARG:C	2:B:606:LYS:N	2.64	0.49
2:B:801:LYS:O	10:J:52:THR:CG2	2.59	0.49
3:C:58:LEU:N	3:C:58:LEU:CD2	2.73	0.49
5:E:100:ILE:HG23	5:E:105:PHE:CD1	2.47	0.49
5:E:73:PRO:HB2	5:E:74:ASP:OD1	2.11	0.49
6:F:99:LEU:HD12	6:F:99:LEU:O	2.13	0.49
8:H:105:GLU:O	8:H:112:ILE:HG23	2.13	0.49
1:A:567:LYS:CD	8:H:95:TYR:HA	2.42	0.49
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.94	0.49
12:L:36:SER:O	12:L:37:LYS:C	2.51	0.49
15:P:6:A:H2'	15:P:7:G:C8	2.46	0.49
1:A:1124:HIS:ND1	1:A:1124:HIS:N	2.60	0.49
1:A:1391:ARG:HG3	1:A:1392:SER:N	2.26	0.49
1:A:159:THR:O	1:A:159:THR:HG22	2.12	0.49
1:A:174:ILE:HG22	1:A:175:ARG:H	1.76	0.49
1:A:189:ARG:O	1:A:190:ALA:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LEU:O	1:A:471:ASN:ND2	2.45	0.49
1:A:964:ILE:O	1:A:967:ALA:HB3	2.12	0.49
2:B:100:PRO:CG	2:B:180:TYR:HE1	2.25	0.49
2:B:278:GLN:CG	2:B:279:ASP:H	2.25	0.49
2:B:461:LEU:N	2:B:461:LEU:HD12	2.27	0.49
2:B:583:ASN:ND2	2:B:628:THR:HG22	2.28	0.49
3:C:132:PRO:O	3:C:133:ILE:C	2.49	0.49
8:H:89:LEU:HB3	8:H:91:ASP:OD1	2.13	0.49
12:L:47:ARG:HH11	12:L:47:ARG:HG3	1.78	0.49
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.53	0.49
1:A:1430:LEU:HB3	1:A:1432:GLN:HG3	1.95	0.49
1:A:202:LEU:HA	1:A:206:GLU:OE1	2.13	0.49
1:A:311:GLN:HB2	1:A:312:PRO:HD3	1.95	0.49
1:A:489:LEU:HD12	1:A:489:LEU:C	2.32	0.49
1:A:524:VAL:HG12	1:A:525:GLN:HG3	1.94	0.49
2:B:36:ALA:HA	2:B:39:ARG:HD2	1.94	0.49
2:B:901:PRO:O	2:B:949:VAL:HB	2.12	0.49
4:D:195:ILE:HG22	4:D:195:ILE:O	2.12	0.49
5:E:197:LYS:CE	5:E:199:ILE:HD11	2.35	0.49
5:E:178:ILE:CG2	5:E:212:ARG:HB3	2.43	0.49
1:A:1280:GLU:O	1:A:1309:ASP:HB3	2.12	0.49
1:A:262:LEU:CD2	1:A:303:TYR:HE1	2.25	0.49
1:A:311:GLN:O	1:A:312:PRO:C	2.50	0.49
1:A:332:LYS:O	1:A:333:GLU:CB	2.60	0.49
1:A:39:GLU:OE1	1:A:50:ILE:HD12	2.13	0.49
1:A:600:PRO:C	1:A:602:ASP:H	2.16	0.49
1:A:745:GLN:N	1:A:748:MET:HE2	2.27	0.49
2:B:258:LEU:O	2:B:258:LEU:CG	2.60	0.49
2:B:44:VAL:O	2:B:45:SER:C	2.51	0.49
2:B:510:LYS:HB2	2:B:511:PRO:HD3	1.94	0.49
2:B:56:ASP:HB2	2:B:57:TYR:HD1	1.77	0.49
2:B:582:VAL:HB	2:B:587:HIS:CD2	2.47	0.49
2:B:616:ILE:HD13	2:B:625:LYS:HB2	1.95	0.49
4:D:203:SER:OG	4:D:206:GLU:HB2	2.13	0.49
4:D:40:HIS:CB	7:G:73:LYS:HZ2	2.26	0.49
1:A:537:ARG:NH1	8:H:120:GLY:O	2.46	0.49
8:H:118:PHE:CZ	8:H:142:LEU:HD22	2.48	0.49
1:A:1100:ARG:HH12	1:A:1111:MET:CE	2.25	0.49
1:A:1344:GLY:O	1:A:1345:ARG:C	2.50	0.49
1:A:390:GLN:O	1:A:394:ASN:CB	2.53	0.49
1:A:567:LYS:CG	1:A:568:PRO:CD	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:LEU:HD21	1:A:1371:LEU:HD22	1.95	0.49
2:B:778:MET:HE2	2:B:1094:ARG:CG	2.43	0.49
2:B:180:TYR:N	2:B:180:TYR:CD1	2.80	0.49
2:B:23:ALA:N	2:B:654:ARG:HB3	2.25	0.49
2:B:734:HIS:O	2:B:735:ALA:HB3	2.13	0.49
2:B:737:THR:CG2	9:I:66:PRO:HA	2.42	0.49
2:B:864:LYS:HD2	2:B:872:GLU:OE2	2.13	0.49
2:B:916:THR:HB	2:B:935:ARG:CG	2.43	0.49
3:C:82:TYR:CE1	3:C:161:LYS:HG2	2.47	0.49
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.94	0.49
5:E:16:PHE:O	5:E:19:VAL:N	2.46	0.49
8:H:101:ALA:HB2	8:H:116:TYR:CZ	2.48	0.49
9:I:44:TYR:CD1	9:I:45:ARG:N	2.80	0.49
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	1.94	0.49
1:A:1226:VAL:HG22	1:A:1240:CYS:HB3	1.95	0.49
1:A:1316:VAL:HG12	1:A:1316:VAL:O	2.13	0.49
1:A:547:LEU:HD22	11:K:58:PHE:HE1	1.73	0.49
1:A:32:VAL:O	1:A:57:ARG:HD3	2.13	0.49
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.53	0.49
1:A:9:ALA:CB	2:B:1193:GLN:HB2	2.43	0.49
2:B:125:SER:HB3	2:B:171:PRO:HA	1.95	0.49
2:B:311:LEU:O	2:B:312:GLU:C	2.51	0.49
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.76	0.49
2:B:821:GLN:NE2	2:B:851:PHE:HA	2.28	0.49
3:C:148:ARG:HG2	3:C:149:LYS:N	2.28	0.49
3:C:98:VAL:O	3:C:99:LEU:HD23	2.13	0.49
6:F:82:THR:HG22	6:F:84:TYR:N	2.23	0.49
4:D:40:HIS:HB2	7:G:73:LYS:CE	2.43	0.49
11:K:18:LYS:HZ3	11:K:38:GLU:HG2	1.76	0.49
1:A:1074:GLU:C	1:A:1076:ALA:N	2.66	0.49
1:A:1451:VAL:C	1:A:1453:TYR:H	2.15	0.49
1:A:187:LYS:O	1:A:188:ASP:HB2	2.13	0.49
1:A:288:ALA:HA	1:A:291:GLU:OE2	2.12	0.49
1:A:364:VAL:O	1:A:364:VAL:HG13	2.12	0.49
1:A:590:ARG:NH1	1:A:590:ARG:CG	2.74	0.49
1:A:591:PHE:HA	1:A:595:THR:CB	2.43	0.49
1:A:753:GLY:HA2	1:A:757:ASN:ND2	2.28	0.49
1:A:86:LEU:HD13	1:A:90:VAL:HG23	1.95	0.49
2:B:171:PRO:HD2	2:B:457:LEU:HD13	1.94	0.49
2:B:172:ILE:HG22	2:B:173:MET:N	2.27	0.49
2:B:190:TYR:CE2	10:J:62:ARG:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:LEU:HD12	2:B:276:ILE:HD12	1.93	0.49
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.35	0.49
2:B:40:GLU:OE1	2:B:682:SER:HB2	2.13	0.49
2:B:873:THR:CG2	2:B:874:PHE:N	2.75	0.49
3:C:41:ILE:CG2	3:C:172:PRO:HG3	2.43	0.49
7:G:88:ASP:CB	7:G:144:ARG:HA	2.39	0.49
8:H:118:PHE:N	8:H:118:PHE:CD1	2.81	0.49
11:K:67:PHE:C	11:K:68:PHE:HD2	2.16	0.49
11:K:55:LYS:HB2	11:K:81:TYR:HE1	1.77	0.49
1:A:1239:ARG:HH11	1:A:1239:ARG:HB3	1.78	0.48
1:A:594:GLY:N	1:A:603:ASN:ND2	2.60	0.48
1:A:83:HIS:CD2	1:A:83:HIS:C	2.87	0.48
1:A:867:ILE:HG22	1:A:872:GLY:N	2.28	0.48
2:B:1002:THR:HG21	2:B:1006:ILE:CG1	2.41	0.48
2:B:1215:ARG:CZ	4:D:15:LEU:HD21	2.43	0.48
2:B:1219:ASP:C	2:B:1219:ASP:OD1	2.52	0.48
2:B:171:PRO:HD2	2:B:457:LEU:HD12	1.94	0.48
2:B:38:PHE:CD1	2:B:811:TYR:CD2	3.01	0.48
2:B:525:ALA:O	2:B:768:THR:HG23	2.13	0.48
2:B:635:ARG:HB2	2:B:636:PRO:CD	2.42	0.48
2:B:651:LEU:C	2:B:653:VAL:H	2.17	0.48
2:B:497:ARG:HH22	2:B:775:LYS:CD	2.26	0.48
2:B:801:LYS:N	10:J:52:THR:CG2	2.75	0.48
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.94	0.48
4:D:56:ARG:CA	4:D:148:LEU:HD13	2.43	0.48
4:D:14:ARG:O	4:D:16:LYS:HG2	2.13	0.48
4:D:214:LEU:O	4:D:218:GLU:HB2	2.13	0.48
5:E:106:GLN:HA	5:E:130:ALA:HB2	1.95	0.48
7:G:132:SER:HB3	7:G:135:ASP:HB2	1.95	0.48
9:I:7:CYS:SG	9:I:8:ARG:O	2.71	0.48
12:L:46:VAL:O	12:L:56:LEU:HD11	2.13	0.48
1:A:186:LYS:O	1:A:187:LYS:CB	2.61	0.48
1:A:231:PRO:C	1:A:233:TRP:H	2.15	0.48
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.48	0.48
1:A:443:LEU:CD1	1:A:455:MET:HB3	2.42	0.48
1:A:491:VAL:HG12	1:A:492:PRO:O	2.13	0.48
1:A:666:ILE:CD1	1:A:667:GLY:N	2.73	0.48
1:A:680:THR:HG23	2:B:729:ILE:CD1	2.43	0.48
1:A:731:ARG:HA	1:A:734:GLU:HB3	1.94	0.48
1:A:914:GLU:HB2	1:A:979:SER:O	2.13	0.48
1:A:9:ALA:O	1:A:10:PRO:C	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1081:LEU:C	2:B:1083:ALA:N	2.65	0.48
2:B:1104:HIS:CG	2:B:1122:ARG:HB2	2.48	0.48
2:B:639:ILE:HG22	2:B:641:GLU:HG2	1.95	0.48
2:B:810:GLU:HA	2:B:815:ARG:NH1	2.28	0.48
2:B:864:LYS:HB2	2:B:872:GLU:CD	2.33	0.48
2:B:918:ILE:HG13	2:B:935:ARG:CZ	2.43	0.48
3:C:164:ALA:HA	3:C:167:HIS:O	2.13	0.48
3:C:179:GLU:HG2	3:C:180:TYR:N	2.28	0.48
3:C:55:THR:O	3:C:56:THR:O	2.31	0.48
4:D:202:ILE:CG2	4:D:207:LEU:HB2	2.43	0.48
6:F:101:ILE:HG23	6:F:107:VAL:HG22	1.94	0.48
6:F:89:GLU:HB3	6:F:134:ILE:HD11	1.95	0.48
7:G:26:LEU:HD12	7:G:56:ILE:HD13	1.95	0.48
12:L:38:LEU:HD13	12:L:49:LYS:HG2	1.94	0.48
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.13	0.48
1:A:598:LEU:O	1:A:598:LEU:HD23	2.14	0.48
1:A:787:PHE:CE1	1:A:796:SER:HA	2.49	0.48
1:A:7:SER:C	1:A:9:ALA:H	2.16	0.48
1:A:889:SER:HB3	1:A:1297:GLU:HG2	1.94	0.48
1:A:913:LEU:HD12	1:A:914:GLU:N	2.28	0.48
2:B:1001:PHE:CD1	2:B:1001:PHE:C	2.87	0.48
2:B:1150:ARG:NH1	2:B:1150:ARG:HB3	2.28	0.48
2:B:411:PRO:O	2:B:414:ALA:HB3	2.13	0.48
2:B:418:LYS:HG2	2:B:422:LYS:HE3	1.96	0.48
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.24	0.48
2:B:681:TRP:HA	2:B:684:LEU:HD12	1.95	0.48
2:B:755:ILE:HG23	2:B:809:MET:HE3	1.95	0.48
2:B:843:GLN:O	2:B:844:SER:C	2.52	0.48
4:D:54:GLU:OE2	4:D:164:ILE:HD11	2.14	0.48
5:E:64:PRO:HB2	5:E:69:ILE:HD11	1.94	0.48
6:F:148:VAL:HG23	6:F:149:GLU:H	1.78	0.48
7:G:6:ASP:HB3	7:G:73:LYS:NZ	2.28	0.48
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.96	0.48
9:I:11:ASN:C	9:I:12:ASN:HD22	2.17	0.48
1:A:1356:ILE:HG21	1:A:1363:VAL:HG21	1.95	0.48
1:A:492:PRO:HB3	1:A:501:LEU:HD12	1.95	0.48
2:B:1068:GLY:O	2:B:1069:PHE:O	2.31	0.48
2:B:22:SER:HA	2:B:654:ARG:CB	2.43	0.48
2:B:435:THR:C	2:B:437:GLU:H	2.16	0.48
2:B:459:TYR:CD2	2:B:459:TYR:C	2.87	0.48
2:B:653:VAL:HG13	2:B:657:HIS:CG	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:SER:HB2	2:B:92:PHE:CD1	2.48	0.48
2:B:821:GLN:NE2	2:B:850:LEU:HD12	2.28	0.48
2:B:895:ASP:C	2:B:897:GLY:H	2.16	0.48
1:A:10:PRO:HA	4:D:1:MET:HB2	1.94	0.48
5:E:22:MET:HE1	5:E:26:ARG:HH11	1.74	0.48
12:L:39:SER:O	12:L:40:LEU:CB	2.60	0.48
12:L:47:ARG:HG2	12:L:52:GLY:O	2.13	0.48
1:A:1142:THR:HB	1:A:1271:ILE:O	2.14	0.48
1:A:1120:LEU:O	1:A:1323:ASP:N	2.47	0.48
1:A:1356:ILE:HG21	1:A:1363:VAL:CG2	2.44	0.48
1:A:963:ILE:HD11	1:A:1048:ASN:HB2	1.95	0.48
2:B:1072:MET:HE2	2:B:1087:PHE:HB2	1.95	0.48
2:B:169:ARG:CB	2:B:454:THR:HG23	2.43	0.48
3:C:160:LYS:O	3:C:161:LYS:O	2.31	0.48
3:C:259:LEU:HD21	11:K:91:CYS:CB	2.41	0.48
3:C:35:ARG:HB3	3:C:35:ARG:HH11	1.78	0.48
5:E:202:SER:HB3	5:E:205:SER:O	2.13	0.48
5:E:78:LEU:HD11	5:E:109:ILE:HD11	1.95	0.48
6:F:89:GLU:HB3	6:F:134:ILE:CD1	2.44	0.48
6:F:74:ILE:CG2	6:F:75:PRO:HD2	2.42	0.48
8:H:40:LEU:HG	8:H:41:ASP:O	2.13	0.48
8:H:41:ASP:O	8:H:42:ILE:HG13	2.14	0.48
8:H:42:ILE:HG22	8:H:44:VAL:HG22	1.95	0.48
9:I:6:PHE:CD1	9:I:11:ASN:OD1	2.64	0.48
11:K:65:HIS:CD2	11:K:67:PHE:N	2.67	0.48
1:A:1005:GLU:O	1:A:1006:ILE:C	2.51	0.48
1:A:105:CYS:SG	1:A:139:TRP:HA	2.54	0.48
1:A:90:VAL:HG11	1:A:297:GLN:HA	1.96	0.48
1:A:353:ILE:HD13	1:A:487:MET:CE	2.40	0.48
1:A:474:VAL:HG22	1:A:474:VAL:O	2.12	0.48
1:A:71:GLN:C	1:A:73:GLY:H	2.16	0.48
1:A:833:GLU:HG2	1:A:1102:LYS:HD2	1.94	0.48
1:A:960:ILE:HA	1:A:963:ILE:CG2	2.43	0.48
2:B:1107:ALA:O	2:B:1108:ARG:HB3	2.13	0.48
1:A:452:LYS:HG3	2:B:1140:ALA:CB	2.44	0.48
5:E:100:ILE:HG23	5:E:105:PHE:CB	2.42	0.48
5:E:77:SER:O	5:E:105:PHE:HB3	2.13	0.48
7:G:15:PRO:CA	7:G:18:PHE:CD1	2.91	0.48
7:G:79:PHE:CE2	7:G:105:PRO:HD2	2.49	0.48
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.95	0.48
13:T:15:DC:H2'	13:T:16:DT:H71	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ALA:O	1:A:83:HIS:HD2	1.97	0.48
1:A:381:THR:HG22	1:A:383:TYR:H	1.79	0.48
1:A:427:GLN:O	1:A:428:TYR:C	2.52	0.48
1:A:915:SER:O	1:A:919:ILE:HG13	2.13	0.48
2:B:1187:ASN:OD1	2:B:1190:ASP:N	2.43	0.48
2:B:181:LEU:CD2	2:B:189:LEU:HD22	2.43	0.48
2:B:213:ILE:HD12	2:B:214:ALA:H	1.78	0.48
2:B:254:LEU:HD11	2:B:273:LEU:HD23	1.96	0.48
2:B:340:ALA:C	2:B:342:GLY:H	2.17	0.48
2:B:600:LEU:O	2:B:609:ILE:HD11	2.14	0.48
1:A:658:LEU:HD12	2:B:830:TYR:CD1	2.49	0.48
3:C:73:GLN:HE21	3:C:74:SER:H	1.62	0.48
4:D:192:LYS:HE3	4:D:204:ASP:OD1	2.14	0.48
5:E:100:ILE:HG23	5:E:105:PHE:CG	2.49	0.48
5:E:2:ASP:O	5:E:3:GLN:HG2	2.14	0.48
9:I:69:PRO:HB2	9:I:85:PHE:HE2	1.77	0.48
11:K:18:LYS:NZ	11:K:37:LYS:O	2.47	0.48
12:L:33:GLU:C	12:L:35:SER:H	2.17	0.48
12:L:58:LYS:HG2	12:L:58:LYS:O	2.12	0.48
1:A:958:VAL:CG2	1:A:1053:PHE:HA	2.44	0.48
1:A:130:ASP:C	1:A:132:LYS:H	2.17	0.48
1:A:540:PHE:HA	1:A:572:TRP:O	2.12	0.48
1:A:608:ILE:C	1:A:610:GLY:N	2.67	0.48
1:A:814:PHE:HE1	2:B:519:TRP:HA	1.77	0.48
1:A:843:LYS:HZ1	2:B:1135:ARG:HH12	1.62	0.48
2:B:274:PRO:O	2:B:275:TYR:HB2	2.13	0.48
2:B:299:GLU:CG	2:B:571:PRO:HG3	2.43	0.48
2:B:589:VAL:CG1	2:B:590:HIS:N	2.75	0.48
2:B:635:ARG:O	2:B:692:TYR:HA	2.13	0.48
2:B:653:VAL:HG13	2:B:657:HIS:CD2	2.48	0.48
2:B:814:PHE:O	2:B:817:LEU:N	2.47	0.48
2:B:855:PHE:CD2	2:B:972:LYS:HE3	2.48	0.48
3:C:33:LEU:HG	3:C:37:MET:CE	2.44	0.48
4:D:163:VAL:O	4:D:166:LEU:HB3	2.13	0.48
5:E:133:GLU:HG2	5:E:135:PHE:HE1	1.79	0.48
5:E:147:HIS:HD2	5:E:149:LEU:H	1.61	0.48
5:E:90:VAL:O	5:E:90:VAL:HG22	2.13	0.48
5:E:91:LYS:C	5:E:93:MET:N	2.65	0.48
6:F:94:LEU:CD2	6:F:122:MET:HA	2.44	0.48
6:F:130:ILE:O	6:F:148:VAL:CG2	2.46	0.48
6:F:135:ARG:NH2	6:F:145:ASP:OD2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001:ARG:HD2	6:F:81:THR:O	2.14	0.48
8:H:56:THR:HB	8:H:145:ARG:HG2	1.96	0.48
3:C:66:ARG:NH2	10:J:2:ILE:CG2	2.76	0.48
10:J:7:CYS:SG	10:J:49:MET:CE	3.02	0.48
11:K:42:LEU:HD22	11:K:71:PHE:HZ	1.79	0.48
11:K:85:ASP:O	11:K:88:LYS:HB2	2.14	0.48
1:A:1273:LEU:CD1	1:A:1273:LEU:N	2.76	0.48
1:A:556:TRP:C	1:A:558:GLY:H	2.16	0.48
1:A:919:ILE:HD13	1:A:983:ILE:CD1	2.44	0.48
2:B:1187:ASN:O	2:B:1188:LYS:CB	2.62	0.48
2:B:743:ILE:N	2:B:743:ILE:HD13	2.28	0.48
2:B:865:LYS:CD	2:B:961:LEU:HD21	2.43	0.48
3:C:29:MET:O	3:C:32:SER:HB2	2.14	0.48
3:C:3:GLU:HB3	11:K:104:ASN:HD21	1.78	0.48
5:E:78:LEU:HD23	5:E:78:LEU:C	2.34	0.48
8:H:107:VAL:HG21	8:H:124:ARG:NH2	2.29	0.48
8:H:142:LEU:C	8:H:143:LEU:HD12	2.34	0.48
8:H:43:ASN:HB3	8:H:95:TYR:OH	2.13	0.48
12:L:38:LEU:HD11	12:L:49:LYS:HE2	1.96	0.48
1:A:1348:LEU:HD21	1:A:1375:MET:SD	2.54	0.48
1:A:1404:GLU:HB3	1:A:1408:ILE:HG13	1.96	0.48
1:A:21:LEU:HD21	1:A:1413:GLY:C	2.34	0.48
1:A:299:HIS:C	1:A:301:ALA:H	2.18	0.48
1:A:308:ILE:HG22	1:A:309:ALA:N	2.19	0.48
1:A:345:VAL:HG23	1:A:346:ASP:O	2.13	0.48
1:A:958:VAL:HG11	1:A:1049:ILE:HG23	1.95	0.48
1:A:971:PHE:C	1:A:973:ILE:H	2.17	0.48
2:B:1156:ASP:O	2:B:1157:ALA:HB3	2.14	0.48
2:B:126:SER:CB	2:B:172:ILE:HD11	2.43	0.48
2:B:361:LEU:N	2:B:362:PRO:CD	2.77	0.48
2:B:67:SER:HB2	2:B:92:PHE:HD1	1.79	0.48
3:C:209:TYR:N	3:C:209:TYR:CD1	2.82	0.48
3:C:77:ILE:HG22	3:C:78:GLU:N	2.29	0.48
4:D:40:HIS:HB3	7:G:73:LYS:NZ	2.28	0.48
6:F:134:ILE:O	6:F:134:ILE:HG22	2.12	0.48
6:F:148:VAL:O	6:F:149:GLU:C	2.51	0.48
6:F:99:LEU:C	6:F:99:LEU:HD12	2.34	0.48
8:H:42:ILE:O	8:H:44:VAL:HG23	2.13	0.48
9:I:19:ASP:OD1	9:I:22:ASN:HB2	2.13	0.48
1:A:1035:TYR:O	1:A:1037:LEU:N	2.46	0.47
1:A:853:ASP:OD1	1:A:855:THR:CG2	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1017:ILE:CB	2:B:1018:PRO:HD3	2.41	0.47
2:B:973:ILE:CG2	2:B:974:PRO:HD2	2.44	0.47
2:B:843:GLN:N	2:B:994:TYR:O	2.31	0.47
3:C:195:GLN:HB3	3:C:196:ASP:H	1.51	0.47
4:D:137:ASN:HD22	4:D:137:ASN:H	1.51	0.47
8:H:100:THR:N	8:H:117:SER:O	2.41	0.47
1:A:323:LYS:H	1:A:323:LYS:CD	2.24	0.47
1:A:347:PHE:HB3	1:A:491:VAL:HB	1.96	0.47
1:A:361:LEU:HA	1:A:471:ASN:ND2	2.29	0.47
1:A:444:PHE:CB	1:A:458:HIS:HD2	2.27	0.47
1:A:500:GLU:O	1:A:504:LEU:HD13	2.14	0.47
1:A:6:TYR:CD1	1:A:7:SER:N	2.82	0.47
1:A:886:ILE:CG2	1:A:952:ALA:HB2	2.44	0.47
2:B:466:TRP:N	2:B:475:SER:HB2	2.29	0.47
2:B:593:PRO:O	2:B:596:LEU:N	2.47	0.47
2:B:616:ILE:H	2:B:616:ILE:HD12	1.79	0.47
2:B:807:ARG:NH1	2:B:807:ARG:HB3	2.28	0.47
2:B:882:THR:HG22	2:B:884:ARG:N	2.29	0.47
6:F:138:LEU:CD2	6:F:139:PRO:HD2	2.43	0.47
7:G:96:GLN:HA	7:G:121:PHE:CZ	2.50	0.47
11:K:24:ASP:H	11:K:31:VAL:HA	1.79	0.47
12:L:55:ILE:HG12	12:L:56:LEU:N	2.28	0.47
13:T:15:DC:H2''	13:T:16:DT:OP2	2.14	0.47
1:A:608:ILE:C	1:A:610:GLY:H	2.16	0.47
1:A:774:ARG:O	1:A:775:ILE:C	2.52	0.47
1:A:784:LEU:C	1:A:786:HIS:H	2.17	0.47
2:B:826:ALA:CB	2:B:1008:PRO:HB3	2.42	0.47
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.96	0.47
2:B:814:PHE:O	2:B:816:GLU:N	2.47	0.47
2:B:880:THR:O	2:B:880:THR:HG22	2.14	0.47
2:B:891:ASP:C	2:B:893:LEU:H	2.16	0.47
3:C:105:GLY:O	3:C:149:LYS:O	2.31	0.47
3:C:124:LEU:HA	3:C:124:LEU:HD23	1.72	0.47
4:D:118:THR:HB	4:D:121:LYS:HB2	1.96	0.47
6:F:119:ARG:O	6:F:122:MET:HB2	2.14	0.47
4:D:23:ASN:O	7:G:83:LYS:HD2	2.14	0.47
8:H:92:ASP:C	8:H:93:TYR:CD1	2.87	0.47
9:I:111:THR:CG2	9:I:113:ASP:HB2	2.45	0.47
11:K:55:LYS:CB	11:K:81:TYR:CE1	2.97	0.47
12:L:31:CYS:HB2	12:L:48:CYS:SG	2.53	0.47
13:T:11:DA:H2''	13:T:12:DG:O5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1114:PRO:O	1:A:1115:SER:O	2.31	0.47
1:A:116:ASP:C	1:A:118:HIS:H	2.16	0.47
1:A:228:PHE:CD2	1:A:228:PHE:N	2.83	0.47
1:A:311:GLN:HB2	1:A:312:PRO:CD	2.44	0.47
1:A:350:ARG:HB2	1:A:488:ASN:OD1	2.15	0.47
1:A:774:ARG:CZ	1:A:797:LYS:CB	2.92	0.47
2:B:1065:GLN:HB3	2:B:1069:PHE:O	2.14	0.47
1:A:7:SER:HB2	2:B:1175:LEU:HD22	1.94	0.47
2:B:286:PHE:HA	2:B:289:LEU:HD12	1.96	0.47
2:B:755:ILE:HG23	2:B:809:MET:HE2	1.96	0.47
2:B:840:ILE:CG2	2:B:994:TYR:HD1	2.26	0.47
2:B:1165:ILE:HG22	4:D:15:LEU:HA	1.97	0.47
5:E:136:ASN:OD1	5:E:137:GLU:N	2.47	0.47
7:G:119:LEU:CD1	7:G:132:SER:HB2	2.44	0.47
7:G:164:LYS:O	7:G:164:LYS:HG2	2.13	0.47
8:H:63:LEU:HD13	8:H:64:ASN:N	2.29	0.47
10:J:25:LEU:O	10:J:29:GLU:HA	2.15	0.47
11:K:55:LYS:HD2	11:K:81:TYR:HD1	1.78	0.47
1:A:1242:VAL:CG1	1:A:1243:VAL:H	2.14	0.47
1:A:265:LYS:O	1:A:269:ILE:HG13	2.14	0.47
1:A:442:VAL:HG11	1:A:489:LEU:HD11	1.97	0.47
1:A:707:GLY:O	1:A:708:MET:HG3	2.14	0.47
2:B:99:LYS:HB3	2:B:100:PRO:HD2	1.96	0.47
2:B:455:SER:O	2:B:458:LYS:HB2	2.13	0.47
2:B:558:LEU:C	2:B:560:GLU:N	2.68	0.47
3:C:176:ILE:CG2	3:C:177:GLU:N	2.78	0.47
1:A:870:GLU:HG2	5:E:208:TYR:CD2	2.49	0.47
6:F:109:VAL:HG11	6:F:123:LYS:CD	2.44	0.47
8:H:86:ASP:O	8:H:87:ARG:O	2.32	0.47
10:J:57:ILE:CA	10:J:60:PHE:HD2	2.24	0.47
1:A:1121:GLU:HB3	1:A:1124:HIS:CD2	2.49	0.47
1:A:326:ARG:NH2	1:A:1407:GLU:HG2	2.29	0.47
1:A:1423:GLY:H	1:A:1426:GLU:HG3	1.80	0.47
1:A:265:LYS:HD3	1:A:303:TYR:CA	2.44	0.47
1:A:384:ASN:O	1:A:385:ILE:C	2.53	0.47
1:A:733:ALA:O	1:A:737:LEU:HG	2.14	0.47
1:A:84:ILE:CG2	1:A:84:ILE:O	2.61	0.47
2:B:1034:VAL:HG21	2:B:1055:ILE:HG23	1.97	0.47
2:B:1047:PHE:N	2:B:1047:PHE:CD1	2.82	0.47
2:B:1065:GLN:NE2	2:B:1067:ARG:H	2.06	0.47
2:B:1112:GLN:HG2	2:B:1113:VAL:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:ILE:O	2:B:278:GLN:N	2.40	0.47
2:B:363:HIS:C	2:B:365:THR:H	2.17	0.47
2:B:891:ASP:O	2:B:893:LEU:N	2.47	0.47
4:D:22:GLU:OE1	4:D:22:GLU:N	2.37	0.47
6:F:79:ARG:HH22	6:F:150:GLU:CD	2.17	0.47
9:I:85:PHE:HD2	9:I:85:PHE:H	1.50	0.47
1:A:709:THR:HG23	9:I:94:ASP:HA	1.97	0.47
1:A:1081:LEU:HD11	1:A:1098:VAL:N	2.25	0.47
1:A:1214:GLU:O	1:A:1218:GLN:HG2	2.15	0.47
1:A:1265:ASN:C	1:A:1267:MET:N	2.66	0.47
1:A:1115:SER:O	1:A:1311:VAL:HG22	2.15	0.47
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.95	0.47
1:A:777:PHE:C	1:A:779:PHE:H	2.16	0.47
2:B:1057:LYS:O	2:B:1061:GLU:HG3	2.14	0.47
3:C:167:HIS:HE1	12:L:70:ARG:HA	1.80	0.47
3:C:233:GLU:HB3	3:C:234:SER:H	1.53	0.47
3:C:43:THR:O	3:C:44:LEU:HB2	2.14	0.47
4:D:29:LEU:HB3	7:G:82:PHE:CE2	2.50	0.47
6:F:73:ALA:HB2	6:F:143:PHE:CD2	2.50	0.47
7:G:112:LYS:O	7:G:115:MET:HG2	2.14	0.47
8:H:103:LYS:HG2	8:H:104:PHE:N	2.30	0.47
1:A:834:THR:HG21	1:A:1077:THR:CB	2.45	0.47
1:A:1360:GLY:O	1:A:1361:SER:O	2.32	0.47
1:A:116:ASP:OD2	1:A:164:ARG:HD2	2.15	0.47
1:A:170:THR:CG2	1:A:171:GLN:N	2.76	0.47
1:A:174:ILE:CG2	1:A:175:ARG:N	2.78	0.47
1:A:477:PRO:HG3	1:A:520:CYS:O	2.15	0.47
1:A:444:PHE:HD1	1:A:489:LEU:HB2	1.80	0.47
1:A:515:GLN:HA	1:A:1367:HIS:NE2	2.30	0.47
1:A:940:ARG:HH11	1:A:940:ARG:HG2	1.80	0.47
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.35	0.47
2:B:352:ALA:HA	2:B:355:ILE:HD12	1.97	0.47
2:B:363:HIS:O	2:B:364:ILE:CB	2.63	0.47
2:B:240:ILE:HG21	2:B:381:MET:HE1	1.95	0.47
4:D:67:ARG:HA	4:D:133:THR:CG2	2.45	0.47
5:E:52:ARG:HG3	5:E:52:ARG:HH11	1.78	0.47
5:E:79:TRP:HE1	5:E:81:GLU:HB2	1.79	0.47
7:G:44:TYR:CD2	7:G:105:PRO:HB2	2.49	0.47
9:I:98:VAL:HG12	9:I:99:LEU:N	2.28	0.47
1:A:203:SER:OG	1:A:206:GLU:HB2	2.15	0.47
1:A:244:PRO:CB	1:A:245:PRO:HD3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ARG:HB3	1:A:469:ARG:HH11	1.80	0.47
1:A:600:PRO:HG2	1:A:601:LYS:N	2.18	0.47
1:A:511:ILE:CG2	1:A:634:THR:HG21	2.44	0.47
1:A:552:TRP:CE3	1:A:651:LYS:HB3	2.50	0.47
1:A:726:ARG:HD2	1:A:765:VAL:O	2.15	0.47
1:A:883:LEU:O	1:A:886:ILE:HG22	2.15	0.47
2:B:29:ASP:CB	2:B:658:ILE:HD13	2.44	0.47
2:B:46:GLN:NE2	2:B:496:ARG:HB3	2.30	0.47
3:C:35:ARG:HD3	11:K:41:THR:HA	1.96	0.47
4:D:119:ARG:HD3	4:D:221:TYR:CD2	2.50	0.47
1:A:1445:ILE:HD13	7:G:70:PHE:CZ	2.50	0.47
8:H:12:VAL:HG13	8:H:26:ILE:HG21	1.96	0.47
11:K:101:LEU:C	11:K:101:LEU:HD23	2.35	0.47
11:K:49:GLU:HA	11:K:52:ASN:ND2	2.30	0.47
13:T:15:DC:C2'	13:T:16:DT:C7	2.88	0.47
1:A:1327:ILE:HG23	5:E:147:HIS:HE1	1.80	0.47
1:A:154:SER:OG	1:A:162:VAL:HG23	2.15	0.47
1:A:541:ILE:HD11	1:A:656:TRP:NE1	2.28	0.47
2:B:1223:ASP:HB3	2:B:1224:PHE:H	1.50	0.47
2:B:269:ILE:HG21	2:B:282:ILE:HD13	1.96	0.47
2:B:435:THR:C	2:B:437:GLU:N	2.68	0.47
2:B:542:MET:CE	2:B:636:PRO:HG3	2.45	0.47
2:B:957:ASN:O	2:B:959:ASP:N	2.48	0.47
5:E:212:ARG:HH11	5:E:212:ARG:HG3	1.79	0.47
6:F:72:LYS:CA	6:F:72:LYS:HE3	2.44	0.47
7:G:88:ASP:HB2	7:G:143:ILE:O	2.15	0.47
7:G:91:VAL:HB	7:G:139:ILE:O	2.13	0.47
8:H:43:ASN:OD1	8:H:46:LEU:N	2.48	0.47
1:A:1058:VAL:O	1:A:1060:PRO:HD3	2.15	0.47
1:A:1284:MET:HA	1:A:1306:LEU:HD23	1.97	0.47
1:A:284:ALA:C	1:A:286:HIS:N	2.65	0.47
1:A:552:TRP:NE1	11:K:62:LYS:HB2	2.30	0.47
1:A:852:TYR:CD2	1:A:1060:PRO:CB	2.96	0.47
2:B:746:SER:HB3	2:B:1046:PRO:CB	2.45	0.47
2:B:54:PHE:CZ	2:B:59:LEU:HD13	2.50	0.47
2:B:687:GLU:O	2:B:689:LEU:N	2.48	0.47
2:B:745:PRO:O	2:B:747:MET:N	2.48	0.47
2:B:195:CYS:HB2	2:B:784:ASN:HB3	1.97	0.47
3:C:221:TYR:CE1	3:C:222:LYS:HG3	2.50	0.47
8:H:116:TYR:HE2	8:H:140:ALA:CB	2.27	0.47
9:I:80:SER:OG	9:I:105:SER:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLU:HG2	1:A:226:GLU:O	2.15	0.46
1:A:299:HIS:O	1:A:301:ALA:N	2.48	0.46
1:A:316:GLN:O	1:A:317:LYS:C	2.53	0.46
1:A:317:LYS:HG2	2:B:471:LYS:NZ	2.29	0.46
1:A:701:LEU:O	1:A:702:LEU:HG	2.14	0.46
1:A:821:ARG:HB2	1:A:821:ARG:NH1	2.30	0.46
1:A:921:GLY:O	1:A:923:LEU:N	2.48	0.46
2:B:1023:VAL:O	2:B:1026:LEU:N	2.48	0.46
2:B:1097:HIS:H	2:B:1098:MET:HE2	1.79	0.46
2:B:170:LEU:O	2:B:172:ILE:N	2.48	0.46
2:B:289:LEU:HD22	2:B:375:ALA:HB2	1.97	0.46
2:B:487:THR:O	2:B:490:SER:HB3	2.15	0.46
2:B:492:LEU:O	2:B:495:LEU:N	2.48	0.46
2:B:687:GLU:CB	2:B:689:LEU:HG	2.44	0.46
2:B:693:ILE:HD13	2:B:701:ILE:HD13	1.97	0.46
3:C:88:CYS:SG	3:C:91:HIS:CA	3.03	0.46
1:A:567:LYS:CB	8:H:96:VAL:H	2.18	0.46
9:I:53:GLY:O	9:I:89:GLN:HB2	2.15	0.46
11:K:44:ASN:N	11:K:61:TYR:CE1	2.83	0.46
1:A:1081:LEU:HD12	1:A:1098:VAL:HG23	1.97	0.46
1:A:1237:ILE:HG22	1:A:1238:ILE:H	1.78	0.46
1:A:482:PHE:N	1:A:482:PHE:CD2	2.80	0.46
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.30	0.46
2:B:26:THR:O	2:B:29:ASP:HB2	2.15	0.46
3:C:169:LYS:HE3	3:C:170:TRP:CZ2	2.50	0.46
5:E:147:HIS:CD2	5:E:149:LEU:H	2.33	0.46
7:G:106:MET:CG	7:G:107:LYS:N	2.78	0.46
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.49	0.46
8:H:110:ASP:O	8:H:128:ASN:HB2	2.15	0.46
8:H:40:LEU:CD1	8:H:123:MET:HB2	2.45	0.46
11:K:78:THR:O	11:K:81:TYR:HB3	2.14	0.46
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.49	0.46
1:A:1002:GLY:CA	1:A:1007:ILE:HG21	2.29	0.46
1:A:1444:MET:O	6:F:132:LEU:HA	2.15	0.46
1:A:693:VAL:O	1:A:693:VAL:HG12	2.15	0.46
1:A:709:THR:HB	1:A:712:GLU:HG3	1.96	0.46
1:A:847:ASP:O	1:A:858:ASN:HA	2.16	0.46
1:A:873:MET:HG3	1:A:1056:SER:O	2.15	0.46
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.44	0.46
2:B:120:ARG:NH1	12:L:54:ARG:HH11	2.13	0.46
2:B:118:ARG:CG	2:B:204:ILE:HD13	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:GLU:O	2:B:315:LYS:HB2	2.15	0.46
2:B:792:MET:HG2	2:B:855:PHE:HE1	1.79	0.46
2:B:896:ASP:OD1	2:B:898:LEU:HB2	2.16	0.46
3:C:11:ARG:NH2	3:C:206:ASN:OD1	2.47	0.46
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.36	0.46
4:D:118:THR:O	4:D:120:GLU:N	2.47	0.46
6:F:96:THR:O	6:F:100:GLN:HG3	2.16	0.46
7:G:88:ASP:HB3	7:G:144:ARG:HB2	1.97	0.46
7:G:96:GLN:HA	7:G:121:PHE:CE2	2.50	0.46
8:H:80:ARG:HH12	11:K:57:LEU:HD11	1.80	0.46
12:L:26:THR:CG2	12:L:27:LEU:N	2.79	0.46
1:A:1067:LEU:O	1:A:1069:ALA:N	2.48	0.46
1:A:1345:ARG:NH1	1:A:1373:ASP:OD1	2.48	0.46
1:A:1423:GLY:CA	1:A:1426:GLU:HG2	2.46	0.46
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.96	0.46
1:A:215:SER:HB3	1:A:218:ASP:CG	2.34	0.46
1:A:269:ILE:HG23	1:A:300:VAL:CG2	2.46	0.46
1:A:332:LYS:HB2	1:A:337:ARG:HD2	1.96	0.46
1:A:402:ALA:HB1	1:A:433:GLU:O	2.16	0.46
1:A:596:THR:C	1:A:598:LEU:N	2.63	0.46
1:A:834:THR:HG21	1:A:1077:THR:CA	2.46	0.46
2:B:768:THR:O	2:B:771:SER:HB2	2.16	0.46
2:B:847:ASP:O	2:B:849:GLY:N	2.49	0.46
3:C:5:GLY:O	3:C:7:GLN:N	2.48	0.46
5:E:129:PRO:O	5:E:130:ALA:O	2.33	0.46
11:K:42:LEU:HD21	11:K:46:ILE:HD12	1.97	0.46
12:L:55:ILE:CG1	12:L:56:LEU:H	2.29	0.46
14:N:5:DC:H2'	14:N:6:DT:H72	1.98	0.46
15:P:6:A:H2'	15:P:7:G:H8	1.80	0.46
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	3.03	0.46
1:A:840:ARG:HH12	1:A:1102:LYS:HE3	1.81	0.46
1:A:1152:ILE:HG22	1:A:1193:LEU:HA	1.96	0.46
1:A:1213:GLY:O	1:A:1216:ILE:N	2.49	0.46
1:A:1371:LEU:O	1:A:1375:MET:HG3	2.14	0.46
1:A:227:VAL:C	1:A:228:PHE:CD2	2.88	0.46
1:A:23:SER:O	1:A:25:GLU:N	2.49	0.46
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.98	0.46
1:A:537:ARG:O	1:A:540:PHE:CE1	2.68	0.46
1:A:542:GLU:O	1:A:546:VAL:HG23	2.16	0.46
1:A:725:ALA:HA	1:A:728:LYS:HE2	1.96	0.46
1:A:901:LEU:HD11	1:A:983:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.50	0.46
2:B:975:GLN:HE22	2:B:1100:ASP:CG	2.18	0.46
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.73	0.46
2:B:388:CYS:O	2:B:390:LEU:N	2.48	0.46
2:B:653:VAL:HA	2:B:657:HIS:CD2	2.50	0.46
2:B:496:ARG:HD2	2:B:751:VAL:CG2	2.45	0.46
2:B:831:SER:HB3	2:B:994:TYR:OH	2.15	0.46
3:C:115:SER:O	3:C:118:LEU:HG	2.15	0.46
3:C:17:ASN:OD1	3:C:233:GLU:HG2	2.15	0.46
3:C:31:ASN:OD1	3:C:34:ARG:HD3	2.16	0.46
5:E:23:VAL:O	5:E:28:TYR:HD1	1.98	0.46
6:F:117:PRO:C	6:F:119:ARG:N	2.69	0.46
8:H:145:ARG:O	8:H:146:ARG:HB2	2.15	0.46
3:C:3:GLU:HG3	11:K:104:ASN:CG	2.35	0.46
2:B:1077:THR:HG22	11:K:44:ASN:HD21	1.81	0.46
1:A:1215:ARG:O	1:A:1218:GLN:HG3	2.16	0.46
1:A:1289:ARG:HH12	1:A:1326:ARG:NH1	2.13	0.46
1:A:1389:PHE:CD1	1:A:1390:ASN:N	2.83	0.46
1:A:1404:GLU:HB2	1:A:1408:ILE:CG1	2.46	0.46
1:A:42:ASP:OD1	1:A:47:ARG:HA	2.15	0.46
1:A:675:THR:HG21	1:A:736:ASN:ND2	2.30	0.46
1:A:829:VAL:O	1:A:832:ALA:N	2.49	0.46
1:A:853:ASP:OD1	1:A:855:THR:N	2.49	0.46
2:B:1069:PHE:CD1	2:B:1069:PHE:N	2.82	0.46
2:B:1098:MET:H	2:B:1098:MET:CE	2.29	0.46
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.45	0.46
2:B:762:ASN:OD1	2:B:1022:THR:HA	2.16	0.46
2:B:955:THR:HG22	2:B:956:THR:N	2.29	0.46
3:C:76:ASP:OD2	3:C:128:ASN:N	2.47	0.46
3:C:167:HIS:CD2	3:C:168:ALA:H	2.32	0.46
3:C:69:LEU:HD12	3:C:69:LEU:N	2.31	0.46
4:D:140:ASP:O	4:D:143:ASN:N	2.49	0.46
4:D:187:THR:HG22	4:D:188:ALA:N	2.31	0.46
4:D:154:PHE:HA	4:D:219:THR:HB	1.98	0.46
5:E:116:ILE:HG22	5:E:117:THR:N	2.31	0.46
6:F:113:GLY:O	6:F:115:THR:HG23	2.15	0.46
8:H:22:LYS:HD3	8:H:45:GLU:OE2	2.16	0.46
8:H:82:PRO:HG3	11:K:54:ARG:CD	2.45	0.46
2:B:785:TYR:HE2	10:J:60:PHE:CE1	2.33	0.46
11:K:20:LYS:HB3	11:K:34:THR:HB	1.97	0.46
1:A:1211:GLN:O	1:A:1212:VAL:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:CYS:C	1:A:144:THR:H	2.18	0.46
1:A:332:LYS:HB2	1:A:337:ARG:NH1	2.30	0.46
1:A:830:LYS:HG3	1:A:1098:VAL:HG11	1.98	0.46
1:A:95:PHE:O	1:A:96:ILE:C	2.54	0.46
2:B:1085:ILE:CD1	2:B:1085:ILE:N	2.74	0.46
2:B:1130:PHE:CE1	2:B:1134:GLU:HB3	2.51	0.46
2:B:213:ILE:HG12	2:B:497:ARG:HB3	1.98	0.46
2:B:69:LEU:HB3	2:B:70:ILE:H	1.63	0.46
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.46	0.46
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.14	0.46
2:B:855:PHE:HD2	2:B:972:LYS:HE3	1.79	0.46
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.30	0.46
3:C:154:LYS:O	3:C:155:LEU:HD23	2.15	0.46
3:C:82:TYR:CE2	3:C:161:LYS:HG2	2.51	0.46
3:C:76:ASP:O	3:C:77:ILE:C	2.54	0.46
4:D:142:LYS:O	4:D:146:GLN:HG3	2.15	0.46
5:E:121:MET:C	5:E:123:LEU:H	2.19	0.46
7:G:137:ILE:CG2	7:G:143:ILE:HD11	2.45	0.46
8:H:113:ALA:HB1	8:H:125:LEU:O	2.16	0.46
10:J:24:LEU:O	10:J:30:LEU:HB2	2.16	0.46
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.97	0.46
1:A:1042:PHE:HE2	1:A:1046:LEU:HD11	1.78	0.46
1:A:877:HIS:CG	1:A:1056:SER:HA	2.51	0.46
1:A:1166:ASP:O	1:A:1167:GLU:C	2.53	0.46
1:A:1325:THR:CG2	1:A:1326:ARG:HG3	2.46	0.46
1:A:367:PRO:HG2	1:A:370:ILE:HD12	1.96	0.46
1:A:432:VAL:HG12	1:A:432:VAL:O	2.15	0.46
1:A:439:ASN:N	1:A:460:VAL:O	2.46	0.46
1:A:553:VAL:HG22	1:A:652:VAL:CG2	2.46	0.46
1:A:52:GLY:N	1:A:56:PRO:HG3	2.31	0.46
1:A:949:ASP:HB3	1:A:951:GLU:H	1.80	0.46
2:B:746:SER:HB3	2:B:1046:PRO:HB2	1.98	0.46
2:B:1072:MET:CE	2:B:1087:PHE:HB2	2.45	0.46
2:B:1181:GLU:N	2:B:1188:LYS:HG3	2.31	0.46
2:B:215:GLN:HA	2:B:215:GLN:NE2	2.31	0.46
2:B:251:ILE:HG22	2:B:251:ILE:O	2.16	0.46
3:C:173:ALA:O	3:C:174:ALA:HB2	2.16	0.46
5:E:100:ILE:O	5:E:100:ILE:CG2	2.63	0.46
5:E:163:GLU:OE2	5:E:167:ARG:HG2	2.15	0.46
6:F:90:ARG:HG3	6:F:91:ALA:H	1.79	0.46
8:H:112:ILE:CG2	8:H:113:ALA:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:50:THR:CG2	9:I:51:ASN:N	2.79	0.46
1:A:1004:ASN:ND2	1:A:1007:ILE:HG12	2.31	0.46
1:A:883:LEU:HD11	1:A:1017:LEU:HD11	1.98	0.46
1:A:1041:ALA:O	1:A:1044:TRP:HB3	2.15	0.46
1:A:1126:ALA:O	1:A:1128:GLN:N	2.49	0.46
1:A:1178:ASP:C	1:A:1179:GLU:HG3	2.36	0.46
1:A:1187:GLN:HA	1:A:1244:ARG:CD	2.45	0.46
1:A:127:ALA:O	1:A:129:LYS:N	2.49	0.46
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.96	0.46
1:A:230:ARG:O	1:A:231:PRO:C	2.54	0.46
1:A:377:PRO:CD	1:A:493:GLN:OE1	2.64	0.46
1:A:575:LYS:HB3	1:A:612:ILE:CG2	2.45	0.46
1:A:618:GLU:O	1:A:620:LYS:N	2.49	0.46
1:A:640:GLN:O	1:A:641:VAL:C	2.53	0.46
1:A:65:LEU:O	1:A:66:LYS:C	2.54	0.46
1:A:726:ARG:HD3	1:A:766:GLY:HA2	1.98	0.46
1:A:786:HIS:CE1	2:B:519:TRP:CZ2	3.02	0.46
2:B:120:ARG:NH1	12:L:54:ARG:NH1	2.64	0.46
2:B:515:HIS:O	2:B:518:HIS:HB2	2.16	0.46
2:B:591:ARG:O	2:B:593:PRO:CD	2.64	0.46
2:B:773:MET:SD	2:B:987:LYS:HE3	2.55	0.46
2:B:794:ASN:O	2:B:795:ILE:HD12	2.15	0.46
2:B:830:TYR:HE2	2:B:1000:PRO:CD	2.22	0.46
2:B:860:MET:HG2	2:B:861:ASP:H	1.78	0.46
1:A:667:GLY:HA3	3:C:192:TRP:CH2	2.50	0.46
3:C:27:LEU:HD11	3:C:178:PHE:HE2	1.80	0.46
9:I:6:PHE:HA	9:I:14:LEU:HG	1.98	0.46
8:H:80:ARG:NH1	11:K:57:LEU:HD11	2.31	0.46
1:A:1308:THR:CG2	1:A:1310:GLY:O	2.63	0.46
1:A:255:SER:OG	2:B:918:ILE:HG23	2.14	0.46
1:A:332:LYS:HA	1:A:337:ARG:HB3	1.98	0.46
1:A:353:ILE:HD11	1:A:480:ALA:HB1	1.97	0.46
1:A:700:ASN:HB2	9:I:98:VAL:CG2	2.46	0.46
1:A:725:ALA:O	1:A:728:LYS:HG2	2.15	0.46
1:A:817:ALA:O	1:A:818:MET:C	2.53	0.46
2:B:1050:ILE:N	2:B:1050:ILE:CD1	2.79	0.46
2:B:244:LEU:HB2	2:B:249:ARG:HA	1.98	0.46
2:B:25:ILE:HG23	2:B:658:ILE:CD1	2.44	0.46
2:B:390:LEU:O	2:B:392:ARG:N	2.48	0.46
2:B:67:SER:O	2:B:68:THR:C	2.54	0.46
2:B:707:PRO:O	2:B:708:GLU:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:857:ARG:O	2:B:967:ARG:HA	2.16	0.46
2:B:859:TYR:H	2:B:859:TYR:HD1	1.62	0.46
2:B:969:ARG:HG2	2:B:970:THR:N	2.31	0.46
3:C:118:LEU:HD12	3:C:132:PRO:HG3	1.98	0.46
3:C:138:GLU:HB2	3:C:140:ASN:ND2	2.31	0.46
3:C:176:ILE:HG22	3:C:177:GLU:O	2.16	0.46
4:D:63:LEU:HD13	4:D:63:LEU:O	2.16	0.46
6:F:138:LEU:HA	6:F:138:LEU:HD23	1.73	0.46
8:H:40:LEU:HD13	8:H:123:MET:SD	2.56	0.46
8:H:131:ASN:C	8:H:133:ASN:H	2.19	0.46
1:A:833:GLU:HG3	1:A:1102:LYS:NZ	2.31	0.45
1:A:1389:PHE:CG	1:A:1390:ASN:N	2.83	0.45
1:A:280:GLU:O	1:A:282:ASN:N	2.48	0.45
1:A:513:SER:OG	1:A:515:GLN:HG2	2.15	0.45
1:A:626:ASN:O	1:A:631:HIS:CD2	2.70	0.45
1:A:666:ILE:CD1	1:A:667:GLY:H	2.13	0.45
1:A:761:MET:HA	1:A:804:TYR:HB2	1.97	0.45
1:A:774:ARG:CZ	1:A:797:LYS:HG3	2.45	0.45
2:B:101:MET:HB3	2:B:109:THR:CG2	2.46	0.45
2:B:435:THR:O	2:B:437:GLU:N	2.49	0.45
2:B:453:ILE:O	2:B:454:THR:C	2.53	0.45
2:B:689:LEU:O	2:B:690:VAL:HG23	2.15	0.45
2:B:879:ARG:HA	2:B:879:ARG:HD3	1.51	0.45
2:B:889:THR:HG23	2:B:891:ASP:OD2	2.16	0.45
3:C:100:THR:HG22	3:C:102:GLN:NE2	2.31	0.45
3:C:147:LEU:HB2	3:C:151:GLN:CB	2.42	0.45
3:C:232:VAL:HG11	3:C:244:VAL:CG2	2.46	0.45
4:D:128:VAL:O	4:D:132:GLN:HG3	2.16	0.45
4:D:192:LYS:HZ3	4:D:199:ASN:HA	1.81	0.45
9:I:19:ASP:HB2	9:I:24:ARG:HG3	1.98	0.45
9:I:72:ASP:HB2	9:I:81:ARG:HB3	1.98	0.45
1:A:1445:ILE:HD12	7:G:59:GLY:O	2.17	0.45
1:A:208:LEU:HD23	1:A:208:LEU:C	2.36	0.45
1:A:507:VAL:HG13	1:A:521:MET:HE1	1.97	0.45
1:A:606:LEU:HD11	1:A:608:ILE:HG13	1.99	0.45
1:A:689:LYS:HE2	1:A:721:PHE:CE2	2.51	0.45
1:A:768:GLN:NE2	1:A:816:HIS:ND1	2.65	0.45
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.51	0.45
1:A:899:VAL:HG22	1:A:908:LEU:HD21	1.98	0.45
2:B:762:ASN:HD21	2:B:1024:ALA:HB3	1.82	0.45
2:B:1084:GLN:C	2:B:1085:ILE:HD12	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:VAL:N	2:B:110:HIS:O	2.44	0.45
2:B:221:ASN:OD1	2:B:242:SER:HA	2.16	0.45
2:B:261:ARG:HH11	2:B:261:ARG:HG3	1.81	0.45
2:B:265:SER:O	2:B:266:ALA:HB3	2.16	0.45
2:B:324:ILE:HG12	2:B:329:THR:HG22	1.98	0.45
2:B:57:TYR:N	2:B:57:TYR:HD1	2.09	0.45
2:B:680:THR:OG1	2:B:681:TRP:N	2.48	0.45
2:B:912:ILE:O	2:B:938:SER:HA	2.16	0.45
2:B:942:ARG:O	2:B:944:THR:N	2.50	0.45
3:C:123:ASN:C	3:C:125:MET:N	2.69	0.45
4:D:16:LYS:C	4:D:18:VAL:H	2.19	0.45
1:A:857:ARG:NH1	6:F:139:PRO:HB2	2.32	0.45
6:F:80:ALA:H	6:F:144:GLU:CD	2.20	0.45
11:K:43:GLY:HA3	11:K:61:TYR:CE1	2.51	0.45
12:L:55:ILE:HG12	12:L:56:LEU:H	1.82	0.45
1:A:1004:ASN:ND2	5:E:167:ARG:CD	2.74	0.45
1:A:146:MET:O	1:A:170:THR:HG23	2.15	0.45
1:A:230:ARG:O	1:A:232:GLU:N	2.49	0.45
1:A:283:GLY:O	1:A:285:PRO:HD3	2.16	0.45
1:A:44:THR:O	1:A:45:GLN:HB2	2.17	0.45
1:A:52:GLY:H	1:A:56:PRO:HG3	1.80	0.45
2:B:1166:CYS:O	2:B:1168:LEU:N	2.41	0.45
2:B:1159:ARG:CD	2:B:1193:GLN:HE21	2.28	0.45
2:B:240:ILE:HG23	2:B:240:ILE:O	2.16	0.45
2:B:253:THR:CG2	2:B:254:LEU:N	2.80	0.45
2:B:261:ARG:NH1	2:B:261:ARG:HG3	2.31	0.45
2:B:383:ASN:O	2:B:387:LEU:HD13	2.16	0.45
2:B:43:LEU:HA	2:B:43:LEU:HD23	1.78	0.45
2:B:779:GLY:O	2:B:795:ILE:HA	2.16	0.45
2:B:858:SER:HA	2:B:966:VAL:O	2.16	0.45
2:B:97:VAL:HG22	2:B:128:LEU:HG	1.97	0.45
3:C:11:ARG:HD3	3:C:209:TYR:OH	2.16	0.45
3:C:238:ILE:CD1	3:C:246:ARG:NH1	2.78	0.45
3:C:77:ILE:O	3:C:79:GLN:N	2.50	0.45
4:D:119:ARG:HD3	4:D:221:TYR:CE2	2.52	0.45
7:G:96:GLN:O	7:G:112:LYS:CD	2.63	0.45
1:A:1120:LEU:CD1	1:A:1120:LEU:H	2.20	0.45
1:A:1127:ASP:HB3	1:A:1130:GLN:HB2	1.99	0.45
1:A:1144:LYS:HD2	1:A:1268:LEU:O	2.17	0.45
1:A:1341:ILE:HG23	1:A:1342:GLU:H	1.82	0.45
1:A:639:PRO:CD	1:A:640:GLN:H	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1087:PHE:CD2	2:B:1087:PHE:C	2.88	0.45
2:B:661:LEU:HD11	2:B:684:LEU:CD1	2.43	0.45
2:B:661:LEU:CD1	2:B:684:LEU:HD11	2.42	0.45
2:B:605:ARG:HB3	2:B:688:GLY:HA2	1.99	0.45
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.46	0.45
2:B:806:THR:HG21	2:B:808:ALA:HB3	1.98	0.45
2:B:815:ARG:O	10:J:54:VAL:HG21	2.16	0.45
2:B:942:ARG:O	2:B:943:SER:C	2.55	0.45
3:C:15:LYS:O	3:C:240:VAL:CG2	2.65	0.45
3:C:17:ASN:N	3:C:240:VAL:HG11	2.32	0.45
4:D:117:GLU:OE2	4:D:155:ARG:O	2.33	0.45
4:D:191:ALA:HB3	4:D:207:LEU:HD21	1.99	0.45
5:E:78:LEU:HD21	5:E:109:ILE:HD12	1.99	0.45
8:H:83:GLN:O	8:H:85:GLY:N	2.49	0.45
9:I:33:SER:O	9:I:35:VAL:HG23	2.16	0.45
2:B:620:ARG:NH2	9:I:89:GLN:HE22	2.15	0.45
14:N:4:DA:H2"	14:N:5:DC:H6	1.81	0.45
1:A:262:LEU:HD12	1:A:328:ARG:NH2	2.32	0.45
1:A:38:PRO:CA	1:A:270:LEU:HD23	2.44	0.45
1:A:300:VAL:O	1:A:300:VAL:HG12	2.16	0.45
1:A:332:LYS:CA	1:A:337:ARG:HB3	2.46	0.45
1:A:777:PHE:C	1:A:779:PHE:N	2.69	0.45
1:A:929:LEU:HD23	1:A:983:ILE:HG21	1.99	0.45
1:A:939:ASP:O	1:A:942:PHE:N	2.46	0.45
2:B:1161:HIS:CE1	2:B:1175:LEU:HD21	2.52	0.45
2:B:287:ARG:NH1	2:B:324:ILE:O	2.49	0.45
2:B:343:ILE:CG2	2:B:347:LYS:HG3	2.47	0.45
2:B:542:MET:HE3	2:B:636:PRO:HG3	1.99	0.45
2:B:63:ILE:O	2:B:67:SER:HB3	2.16	0.45
2:B:751:VAL:HG13	2:B:812:LEU:HD22	1.99	0.45
2:B:766:ARG:HH21	15:P:11:U:H3	1.65	0.45
2:B:529:GLU:OE2	2:B:769:TYR:CD1	2.70	0.45
2:B:911:ILE:O	2:B:911:ILE:HG22	2.16	0.45
3:C:168:ALA:O	3:C:171:GLY:N	2.47	0.45
3:C:49:VAL:HG21	3:C:64:ALA:HA	1.98	0.45
4:D:51:ASN:OD1	4:D:54:GLU:CB	2.65	0.45
5:E:172:GLU:HG3	5:E:213:ILE:CD1	2.47	0.45
5:E:60:PHE:CD2	5:E:60:PHE:C	2.88	0.45
7:G:119:LEU:HA	7:G:131:GLN:O	2.16	0.45
8:H:59:ILE:HG12	8:H:142:LEU:HD12	1.96	0.45
1:A:560:ILE:CD1	8:H:79:TRP:HB3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:9:ILE:HG12	8:H:56:THR:HA	1.98	0.45
9:I:99:LEU:C	9:I:100:PHE:CD1	2.90	0.45
10:J:53:HIS:CE1	10:J:55:ASP:HA	2.51	0.45
12:L:32:ALA:H	12:L:55:ILE:HG13	1.82	0.45
1:A:836:TYR:HB2	13:T:18:DA:H5'	1.97	0.45
1:A:1017:LEU:O	1:A:1017:LEU:HD12	2.16	0.45
1:A:1259:MET:HG3	1:A:1262:LYS:NZ	2.28	0.45
1:A:1341:ILE:HD12	1:A:1379:GLY:O	2.17	0.45
1:A:347:PHE:CD1	1:A:347:PHE:N	2.85	0.45
1:A:783:THR:O	1:A:784:LEU:HD23	2.16	0.45
2:B:120:ARG:NE	2:B:955:THR:CG2	2.74	0.45
2:B:282:ILE:HD11	2:B:317:CYS:SG	2.56	0.45
2:B:365:THR:HG23	2:B:367:LEU:N	2.30	0.45
2:B:766:ARG:HD3	2:B:766:ARG:HA	1.80	0.45
2:B:801:LYS:O	2:B:822:ASN:ND2	2.50	0.45
2:B:936:ASP:OD1	2:B:937:ALA:N	2.49	0.45
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.98	0.45
5:E:42:PHE:HZ	5:E:58:MET:CE	2.29	0.45
7:G:138:THR:CG2	7:G:139:ILE:N	2.60	0.45
8:H:130:ARG:N	8:H:130:ARG:CD	2.74	0.45
9:I:7:CYS:O	9:I:8:ARG:O	2.34	0.45
10:J:56:LEU:O	10:J:59:LYS:N	2.50	0.45
11:K:55:LYS:HB3	11:K:81:TYR:CE1	2.51	0.45
1:A:1123:GLY:O	1:A:1125:ALA:N	2.49	0.45
1:A:134:ARG:HG2	1:A:138:ILE:HD11	1.99	0.45
1:A:95:PHE:HD1	1:A:234:MET:HA	1.82	0.45
1:A:452:LYS:HE3	2:B:1141:HIS:ND1	2.32	0.45
1:A:49:LYS:NZ	1:A:61:ILE:CG1	2.78	0.45
1:A:562:THR:HA	1:A:563:PRO:HD3	1.79	0.45
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.63	0.45
1:A:971:PHE:HE2	1:A:1040:GLN:HG2	1.82	0.45
2:B:1002:THR:O	2:B:1003:ALA:C	2.55	0.45
2:B:100:PRO:CD	2:B:180:TYR:HE1	2.29	0.45
1:A:1431:GLY:HA3	2:B:1152:MET:SD	2.56	0.45
2:B:582:VAL:HG22	2:B:626:ILE:HG21	1.99	0.45
2:B:58:THR:O	2:B:62:ILE:HG13	2.17	0.45
2:B:640:VAL:HG23	2:B:740:HIS:HA	1.99	0.45
2:B:658:ILE:HG22	2:B:659:ALA:N	2.32	0.45
2:B:616:ILE:HG13	2:B:697:GLU:HA	1.98	0.45
3:C:114:TYR:HB3	3:C:140:ASN:O	2.17	0.45
4:D:130:LEU:HD13	4:D:142:LYS:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.97	0.45
5:E:147:HIS:O	5:E:148:GLU:C	2.55	0.45
5:E:202:SER:C	5:E:204:THR:H	2.19	0.45
5:E:46:TYR:CE2	5:E:58:MET:HA	2.51	0.45
7:G:20:PRO:HG2	7:G:21:ARG:H	1.81	0.45
1:A:834:THR:HG21	1:A:1077:THR:CG2	2.46	0.45
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.99	0.45
1:A:12:ARG:HD2	2:B:1218:THR:CB	2.43	0.45
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.99	0.45
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.99	0.45
1:A:850:VAL:HG21	1:A:1058:VAL:HG11	1.99	0.45
1:A:883:LEU:CD2	1:A:1021:LEU:HB2	2.46	0.45
1:A:902:LEU:HD11	1:A:923:LEU:CD2	2.44	0.45
2:B:1112:GLN:HG2	2:B:1113:VAL:H	1.81	0.45
2:B:1171:VAL:HA	2:B:1182:CYS:HB2	1.99	0.45
2:B:211:VAL:HG12	2:B:211:VAL:O	2.16	0.45
2:B:234:ILE:CG2	2:B:235:SER:N	2.79	0.45
2:B:515:HIS:CD2	2:B:516:ASN:H	2.34	0.45
2:B:611:PRO:HB3	2:B:685:LEU:CD1	2.47	0.45
2:B:638:PHE:CA	2:B:690:VAL:HG22	2.23	0.45
2:B:755:ILE:HG22	2:B:755:ILE:O	2.17	0.45
2:B:995:ARG:HH12	3:C:165:LYS:HG2	1.82	0.45
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.98	0.45
4:D:8:PHE:CD2	7:G:6:ASP:O	2.70	0.45
5:E:73:PRO:HB2	5:E:74:ASP:H	1.61	0.45
8:H:64:ASN:CB	8:H:88:SER:HB2	2.34	0.45
9:I:1:MET:CE	9:I:4:PHE:HB3	2.46	0.45
9:I:1:MET:HE1	9:I:4:PHE:HD2	1.82	0.45
1:A:1259:MET:HA	1:A:1262:LYS:HG3	1.98	0.45
1:A:270:LEU:O	1:A:273:ASN:HB3	2.17	0.45
1:A:332:LYS:CG	1:A:333:GLU:HG2	2.46	0.45
1:A:600:PRO:HA	8:H:25:ARG:NH2	2.31	0.45
1:A:722:LEU:H	1:A:722:LEU:HD12	1.82	0.45
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.97	0.45
1:A:76:GLU:O	1:A:78:PRO:CD	2.65	0.45
1:A:767:GLN:NE2	1:A:774:ARG:HB2	2.32	0.45
2:B:128:LEU:HB2	2:B:167:ILE:O	2.17	0.45
2:B:653:VAL:HG22	2:B:689:LEU:HD22	1.99	0.45
2:B:899:ILE:HG23	2:B:903:VAL:HG21	1.97	0.45
3:C:65:HIS:O	3:C:69:LEU:HD13	2.17	0.45
4:D:119:ARG:CG	4:D:221:TYR:HE2	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:55:ALA:HB3	4:D:148:LEU:HD11	1.98	0.45
4:D:41:GLN:HA	4:D:41:GLN:OE1	2.17	0.45
7:G:115:MET:SD	7:G:119:LEU:HD23	2.56	0.45
4:D:7:THR:HB	7:G:42:PHE:CE2	2.52	0.45
8:H:5:LEU:CD1	8:H:135:LEU:HD12	2.47	0.45
13:T:20:DG:H2''	13:T:21:DC:H5'	1.99	0.45
1:A:106:VAL:HG12	1:A:107:CYS:N	2.32	0.45
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.17	0.45
1:A:1237:ILE:CG2	1:A:1238:ILE:H	2.30	0.45
1:A:1293:SER:HB2	1:A:1299:VAL:CG2	2.47	0.45
1:A:1377:THR:O	1:A:1378:GLN:C	2.55	0.45
1:A:1395:GLY:HA3	1:A:1419:ASP:OD2	2.16	0.45
1:A:162:VAL:HG12	1:A:163:SER:N	2.32	0.45
1:A:225:ASN:HD22	1:A:228:PHE:H	1.56	0.45
1:A:40:THR:HB	1:A:41:MET:HE3	1.97	0.45
1:A:507:VAL:N	1:A:508:PRO:CD	2.79	0.45
1:A:567:LYS:HE2	8:H:46:LEU:O	2.17	0.45
1:A:880:LYS:HA	1:A:954:TRP:O	2.17	0.45
1:A:896:ARG:HH21	1:A:1030:ARG:CZ	2.29	0.45
2:B:953:LEU:H	2:B:953:LEU:HD23	1.81	0.45
3:C:239:PRO:O	3:C:241:ASP:N	2.50	0.45
5:E:186:LEU:O	5:E:187:TYR:C	2.55	0.45
5:E:90:VAL:O	5:E:93:MET:HB3	2.17	0.45
6:F:99:LEU:HD21	7:G:64:THR:O	2.16	0.45
11:K:78:THR:O	11:K:79:GLU:O	2.35	0.45
12:L:52:GLY:O	12:L:54:ARG:N	2.50	0.45
1:A:1152:ILE:CG2	1:A:1193:LEU:HD13	2.46	0.44
1:A:153:PRO:HA	1:A:161:LEU:HA	1.99	0.44
1:A:326:ARG:CG	1:A:327:ALA:N	2.78	0.44
1:A:464:PRO:HG2	1:A:465:TYR:CD1	2.52	0.44
1:A:52:GLY:C	1:A:56:PRO:HG2	2.37	0.44
1:A:755:PHE:HA	1:A:758:ILE:HD12	1.98	0.44
1:A:932:GLU:O	1:A:936:LEU:HG	2.17	0.44
1:A:942:PHE:C	1:A:942:PHE:CD2	2.91	0.44
1:A:946:VAL:C	1:A:947:PHE:HD1	2.20	0.44
2:B:1034:VAL:C	2:B:1036:ALA:N	2.71	0.44
2:B:1150:ARG:NH1	2:B:1150:ARG:HG3	2.18	0.44
2:B:116:GLU:C	2:B:118:ARG:N	2.71	0.44
2:B:344:LYS:O	2:B:345:LYS:O	2.34	0.44
2:B:313:MET:CE	2:B:386:LEU:HD22	2.47	0.44
2:B:461:LEU:CD1	2:B:461:LEU:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:ILE:H	3:C:38:ILE:HG13	1.44	0.44
1:A:1325:THR:OG1	5:E:146:HIS:O	2.33	0.44
1:A:1339:LEU:O	5:E:183:PRO:HB2	2.16	0.44
5:E:23:VAL:HB	5:E:30:ILE:HD11	1.99	0.44
5:E:78:LEU:HD21	5:E:80:VAL:HG23	1.98	0.44
7:G:154:VAL:HG12	7:G:155:SER:N	2.32	0.44
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.99	0.44
8:H:64:ASN:HA	8:H:90:ALA:HB2	1.99	0.44
1:A:1161:THR:CG2	1:A:1163:ILE:HG13	2.45	0.44
1:A:202:LEU:HD13	1:A:207:ILE:HD11	1.99	0.44
1:A:75:ASN:O	1:A:76:GLU:HB2	2.17	0.44
2:B:1050:ILE:HG22	2:B:1051:THR:N	2.33	0.44
1:A:18:GLN:CB	2:B:1215:ARG:HB2	2.47	0.44
2:B:460:ALA:HB1	2:B:466:TRP:CE3	2.53	0.44
2:B:649:LYS:HD3	2:B:736:THR:O	2.16	0.44
2:B:846:ILE:CG2	2:B:974:PRO:HG2	2.47	0.44
3:C:99:LEU:HD23	3:C:99:LEU:N	2.31	0.44
4:D:39:ASN:HD22	4:D:41:GLN:HB2	1.82	0.44
6:F:79:ARG:HH11	6:F:79:ARG:CG	2.28	0.44
7:G:145:VAL:HG12	7:G:146:LYS:H	1.81	0.44
8:H:100:THR:CB	8:H:138:GLU:HG3	2.47	0.44
9:I:55:THR:HG23	9:I:86:PHE:CZ	2.52	0.44
11:K:90:ALA:O	11:K:93:SER:HB3	2.17	0.44
1:A:332:LYS:CB	1:A:337:ARG:HD2	2.47	0.44
1:A:478:TYR:O	1:A:479:ASN:CB	2.65	0.44
1:A:637:LYS:HG3	1:A:641:VAL:HG11	1.98	0.44
1:A:630:ILE:CD1	1:A:646:PHE:CZ	2.99	0.44
1:A:754:SER:O	1:A:755:PHE:C	2.55	0.44
1:A:874:ASP:O	1:A:876:ALA:N	2.51	0.44
2:B:1152:MET:C	2:B:1157:ALA:HB2	2.38	0.44
2:B:306:ASN:C	2:B:308:TRP:H	2.21	0.44
2:B:601:ARG:C	2:B:603:LEU:N	2.70	0.44
2:B:830:TYR:CE2	2:B:1000:PRO:CD	2.97	0.44
3:C:112:ASN:HB3	3:C:114:TYR:CE1	2.52	0.44
3:C:138:GLU:OE1	3:C:138:GLU:N	2.50	0.44
5:E:10:SER:O	5:E:13:TRP:HB3	2.17	0.44
8:H:106:GLU:O	8:H:108:SER:N	2.50	0.44
8:H:64:ASN:ND2	8:H:88:SER:C	2.71	0.44
9:I:4:PHE:HD1	9:I:5:ARG:N	2.15	0.44
10:J:9:SER:CB	10:J:45:CYS:HB2	2.47	0.44
13:T:8:DT:H2"	13:T:9:DC:OP2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1095:THR:HG22	1:A:1100:ARG:HB2	2.00	0.44
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.99	0.44
1:A:1239:ARG:HB3	1:A:1239:ARG:NH1	2.32	0.44
1:A:1244:ARG:CB	1:A:1245:PRO:CA	2.86	0.44
1:A:1072:ILE:HG23	1:A:1356:ILE:HD11	1.99	0.44
1:A:293:GLU:O	1:A:296:LEU:N	2.48	0.44
1:A:54:ASN:C	1:A:56:PRO:HD3	2.38	0.44
1:A:682:THR:HG23	1:A:728:LYS:HE3	1.98	0.44
1:A:784:LEU:HB3	1:A:785:PRO:HD2	1.99	0.44
2:B:1045:SER:O	2:B:1046:PRO:O	2.36	0.44
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.97	0.44
2:B:451:LYS:O	2:B:455:SER:OG	2.32	0.44
2:B:834:ASN:HA	2:B:839:MET:HA	1.98	0.44
2:B:953:LEU:N	2:B:953:LEU:HD23	2.33	0.44
4:D:7:THR:HB	7:G:42:PHE:HE2	1.83	0.44
14:N:3:DT:OP2	14:N:3:DT:H3'	2.17	0.44
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.16	0.44
1:A:1159:ARG:O	1:A:1160:SER:HB3	2.17	0.44
1:A:1278:ASN:HD22	1:A:1312:ASN:HB2	1.81	0.44
1:A:1289:ARG:NH1	1:A:1326:ARG:NH1	2.65	0.44
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.98	0.44
1:A:278:THR:O	1:A:278:THR:HG22	2.17	0.44
1:A:299:HIS:C	1:A:301:ALA:N	2.71	0.44
1:A:630:ILE:CG2	1:A:631:HIS:N	2.80	0.44
1:A:645:LEU:CG	1:A:649:ILE:HD11	2.48	0.44
2:B:1115:THR:CG2	2:B:1117:GLN:HG3	2.42	0.44
1:A:22:PHE:CE1	2:B:1213:THR:HG22	2.52	0.44
2:B:797:TYR:CE1	2:B:971:THR:HG23	2.53	0.44
2:B:801:LYS:HD2	2:B:815:ARG:HB3	1.99	0.44
2:B:877:PRO:HB2	2:B:934:LYS:HD2	2.00	0.44
2:B:997:GLU:HB3	3:C:35:ARG:NH1	2.32	0.44
3:C:172:PRO:CD	3:C:173:ALA:H	2.31	0.44
3:C:20:PHE:CZ	3:C:230:MET:HB2	2.53	0.44
3:C:77:ILE:C	3:C:79:GLN:H	2.21	0.44
4:D:145:MET:O	4:D:149:THR:N	2.50	0.44
4:D:166:LEU:HD11	4:D:210:ILE:HG23	1.99	0.44
4:D:18:VAL:O	4:D:19:GLU:CB	2.58	0.44
4:D:60:LYS:HE3	4:D:126:ILE:HD11	1.99	0.44
9:I:1:MET:HE1	9:I:4:PHE:CD2	2.53	0.44
10:J:56:LEU:O	10:J:57:ILE:C	2.54	0.44
13:T:11:DA:C2	13:T:12:DG:C4	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1259:MET:HG3	1:A:1262:LYS:CE	2.48	0.44
1:A:1364:ASN:O	1:A:1365:TYR:C	2.56	0.44
1:A:1398:MET:O	1:A:1400:CYS:N	2.50	0.44
1:A:275:SER:O	1:A:279:LEU:HG	2.17	0.44
1:A:341:MET:CE	2:B:1135:ARG:NH1	2.80	0.44
2:B:20:ASP:C	2:B:22:SER:N	2.68	0.44
2:B:684:LEU:HD23	2:B:689:LEU:HD12	1.99	0.44
2:B:705:MET:CE	2:B:742:GLU:HG2	2.48	0.44
2:B:496:ARG:HD2	2:B:751:VAL:HG23	2.00	0.44
3:C:235:VAL:HG11	10:J:6:ARG:NH2	2.32	0.44
9:I:105:SER:O	9:I:106:CYS:CB	2.59	0.44
13:T:25:DG:H2''	13:T:26:DT:H5'	1.99	0.44
1:A:101:LYS:HA	1:A:104:GLU:OE1	2.17	0.44
1:A:1127:ASP:CB	1:A:1130:GLN:HB2	2.47	0.44
1:A:1271:ILE:HG22	1:A:1271:ILE:O	2.16	0.44
1:A:1272:THR:HG22	1:A:1273:LEU:N	2.32	0.44
1:A:230:ARG:O	1:A:233:TRP:N	2.51	0.44
1:A:442:VAL:CG2	1:A:460:VAL:HG23	2.48	0.44
1:A:54:ASN:CB	1:A:247:ARG:HH22	2.31	0.44
1:A:682:THR:HG22	1:A:728:LYS:HE3	1.98	0.44
1:A:72:GLU:HB3	1:A:76:GLU:CG	2.45	0.44
2:B:189:LEU:O	2:B:192:LEU:N	2.50	0.44
2:B:348:ARG:O	2:B:351:TYR:HB3	2.18	0.44
2:B:357:GLN:HG2	2:B:366:GLN:O	2.17	0.44
2:B:388:CYS:C	2:B:390:LEU:H	2.21	0.44
2:B:213:ILE:HD11	2:B:497:ARG:CA	2.48	0.44
2:B:616:ILE:HD12	2:B:625:LYS:HB2	1.99	0.44
2:B:870:ILE:CG2	2:B:917:PRO:HG2	2.48	0.44
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.47	0.44
4:D:126:ILE:HD13	4:D:145:MET:HE3	2.00	0.44
5:E:154:ILE:HG22	5:E:155:ARG:O	2.17	0.44
5:E:50:MET:HE2	5:E:50:MET:N	2.32	0.44
7:G:17:PHE:O	7:G:19:GLY:N	2.44	0.44
9:I:69:PRO:HG2	9:I:85:PHE:CE2	2.52	0.44
1:A:1115:SER:O	1:A:1116:LEU:CB	2.65	0.44
1:A:1138:ILE:C	1:A:1275:GLY:HA2	2.37	0.44
1:A:1170:ILE:HG13	1:A:1170:ILE:H	1.62	0.44
1:A:1291:VAL:HG13	1:A:1292:PRO:N	2.33	0.44
1:A:208:LEU:HD21	1:A:212:LYS:HE3	1.99	0.44
1:A:407:ARG:HB3	1:A:430:TRP:CZ2	2.53	0.44
1:A:40:THR:CG2	1:A:41:MET:HE2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:914:GLU:C	1:A:916:GLY:H	2.22	0.44
2:B:1004:GLU:HB2	2:B:1006:ILE:HG12	1.98	0.44
2:B:266:ALA:C	2:B:268:THR:H	2.18	0.44
2:B:305:VAL:HG12	2:B:305:VAL:O	2.18	0.44
2:B:803:LEU:CD1	2:B:1032:SER:HB3	2.48	0.44
3:C:67:LEU:HD23	3:C:70:ILE:CD1	2.47	0.44
3:C:87:PHE:CD1	3:C:87:PHE:N	2.85	0.44
5:E:121:MET:O	5:E:124:VAL:HG23	2.18	0.44
5:E:95:THR:O	5:E:99:HIS:HB2	2.17	0.44
6:F:114:GLU:HA	6:F:114:GLU:OE2	2.18	0.44
6:F:116:ASP:HB3	6:F:119:ARG:HB2	2.00	0.44
6:F:84:TYR:CD2	6:F:152:ILE:HB	2.52	0.44
7:G:27:LYS:O	7:G:31:LEU:HG	2.17	0.44
8:H:100:THR:CG2	8:H:101:ALA:N	2.80	0.44
8:H:84:ALA:HA	8:H:87:ARG:HG3	2.00	0.44
10:J:27:GLU:C	10:J:29:GLU:N	2.71	0.44
11:K:1:MET:HG3	11:K:2:ASN:N	2.33	0.44
12:L:34:CYS:O	12:L:35:SER:C	2.55	0.44
12:L:38:LEU:O	12:L:39:SER:HB3	2.18	0.44
1:A:1021:LEU:O	1:A:1024:SER:HB3	2.18	0.44
1:A:1436:ILE:O	1:A:1437:GLY:C	2.56	0.44
1:A:157:ASP:C	1:A:159:THR:N	2.71	0.44
1:A:23:SER:HA	1:A:233:TRP:CD1	2.53	0.44
1:A:577:ILE:HA	1:A:580:VAL:HG23	1.99	0.44
1:A:64:ASN:O	1:A:65:LEU:C	2.55	0.44
1:A:767:GLN:HE21	1:A:774:ARG:CB	2.31	0.44
1:A:853:ASP:OD1	1:A:855:THR:CB	2.66	0.44
2:B:186:GLU:OE2	2:B:186:GLU:HA	2.17	0.44
2:B:361:LEU:O	2:B:363:HIS:O	2.36	0.44
2:B:737:THR:HG22	9:I:66:PRO:HA	2.00	0.44
3:C:184:ASN:HD21	3:C:187:LYS:HA	1.79	0.44
3:C:215:GLU:O	3:C:217:ASP:N	2.50	0.44
4:D:155:ARG:CG	4:D:155:ARG:HH11	2.28	0.44
5:E:177:ARG:C	5:E:212:ARG:HD3	2.38	0.44
6:F:94:LEU:HD21	6:F:122:MET:HA	2.00	0.44
10:J:37:SER:OG	10:J:47:ARG:NH2	2.49	0.44
1:A:552:TRP:HE1	11:K:62:LYS:HB2	1.83	0.44
12:L:61:THR:HG22	12:L:62:LYS:N	2.33	0.44
1:A:1220:PHE:O	1:A:1221:LYS:CB	2.65	0.43
1:A:1230:GLU:C	1:A:1232:ASN:N	2.71	0.43
1:A:22:PHE:HE2	1:A:30:ILE:CD1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ASN:O	1:A:343:LYS:HG2	2.17	0.43
1:A:456:MET:HB2	1:A:478:TYR:OH	2.17	0.43
1:A:606:LEU:CG	1:A:613:ILE:HD12	2.47	0.43
1:A:817:ALA:O	1:A:819:GLY:N	2.50	0.43
2:B:999:MET:CG	2:B:1000:PRO:HD2	2.24	0.43
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.53	0.43
2:B:854:LEU:HB3	2:B:855:PHE:H	1.70	0.43
2:B:843:GLN:HB3	2:B:995:ARG:HG3	2.00	0.43
4:D:191:ALA:C	4:D:193:THR:H	2.21	0.43
4:D:218:GLU:O	4:D:219:THR:C	2.56	0.43
6:F:72:LYS:HB3	6:F:73:ALA:H	1.53	0.43
7:G:115:MET:HB2	7:G:116:PRO:CD	2.43	0.43
8:H:42:ILE:HG22	8:H:44:VAL:CG2	2.48	0.43
8:H:64:ASN:OD1	8:H:90:ALA:N	2.35	0.43
1:A:1164:PRO:C	1:A:1166:ASP:N	2.71	0.43
1:A:1164:PRO:O	1:A:1166:ASP:N	2.51	0.43
1:A:133:LYS:O	1:A:136:ALA:HB3	2.18	0.43
1:A:332:LYS:O	1:A:333:GLU:HB2	2.17	0.43
1:A:899:VAL:CG2	1:A:908:LEU:HD21	2.48	0.43
2:B:1084:GLN:NE2	2:B:1084:GLN:H	2.13	0.43
2:B:270:LYS:HG2	2:B:281:PRO:HA	2.00	0.43
2:B:258:LEU:HB2	2:B:385:LEU:HD21	2.00	0.43
2:B:39:ARG:CZ	2:B:665:GLU:HG2	2.49	0.43
2:B:416:LEU:HD11	2:B:466:TRP:CE2	2.53	0.43
2:B:436:VAL:O	2:B:436:VAL:HG12	2.17	0.43
2:B:68:THR:HG22	2:B:69:LEU:N	2.32	0.43
3:C:123:ASN:ND2	3:C:125:MET:HA	2.32	0.43
3:C:220:ASP:OD1	3:C:223:ALA:N	2.51	0.43
3:C:58:LEU:HD22	3:C:58:LEU:H	1.78	0.43
4:D:39:ASN:O	4:D:42:GLY:N	2.50	0.43
7:G:127:PRO:HB3	7:G:139:ILE:HD11	2.00	0.43
9:I:7:CYS:C	9:I:8:ARG:O	2.56	0.43
11:K:88:LYS:O	11:K:91:CYS:HB2	2.18	0.43
1:A:116:ASP:O	1:A:118:HIS:N	2.52	0.43
1:A:1430:LEU:CB	1:A:1432:GLN:HG3	2.48	0.43
1:A:184:SER:HB3	1:A:199:LEU:CD2	2.47	0.43
1:A:239:LEU:HA	1:A:240:PRO:HD2	1.86	0.43
1:A:179:LEU:HD13	1:A:297:GLN:HG3	2.00	0.43
1:A:402:ALA:CB	1:A:434:ARG:HA	2.49	0.43
1:A:453:MET:HE3	1:A:513:SER:HB2	2.01	0.43
1:A:445:ASN:HB2	1:A:454:SER:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.53	0.43
1:A:682:THR:HG22	1:A:682:THR:O	2.18	0.43
1:A:858:ASN:ND2	1:A:858:ASN:C	2.72	0.43
1:A:947:PHE:HE2	1:A:954:TRP:CD1	2.36	0.43
2:B:204:ILE:C	2:B:205:ILE:HD12	2.39	0.43
2:B:370:PHE:HE2	2:B:373:ARG:NH1	2.16	0.43
2:B:766:ARG:HA	2:B:769:TYR:HD2	1.82	0.43
4:D:37:GLN:OE1	7:G:5:LYS:HD2	2.18	0.43
5:E:178:ILE:HG22	5:E:212:ARG:HB3	2.01	0.43
5:E:7:ARG:HD2	5:E:7:ARG:C	2.38	0.43
7:G:13:LEU:HD22	7:G:14:HIS:O	2.17	0.43
1:A:1130:GLN:HE21	1:A:1134:ILE:HD11	1.83	0.43
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.58	0.43
1:A:295:LEU:O	1:A:298:PHE:HB3	2.18	0.43
1:A:55:ASP:N	1:A:56:PRO:CD	2.80	0.43
1:A:727:ASP:O	1:A:730:GLY:N	2.51	0.43
1:A:941:LYS:O	1:A:945:GLU:HB2	2.18	0.43
2:B:1002:THR:O	2:B:1004:GLU:N	2.52	0.43
2:B:1099:VAL:O	2:B:1101:ASP:N	2.52	0.43
2:B:510:LYS:CB	2:B:511:PRO:CD	2.96	0.43
2:B:572:HIS:O	2:B:573:GLN:C	2.56	0.43
2:B:597:MET:HE2	2:B:597:MET:HA	1.99	0.43
2:B:889:THR:HG22	2:B:891:ASP:HB2	2.01	0.43
3:C:22:LEU:HD23	3:C:23:SER:N	2.34	0.43
3:C:46:ILE:HD12	3:C:67:LEU:O	2.17	0.43
4:D:56:ARG:HH21	4:D:155:ARG:HA	1.83	0.43
4:D:170:THR:HG22	4:D:172:LEU:HG	2.00	0.43
5:E:11:ARG:C	5:E:13:TRP:N	2.70	0.43
5:E:173:SER:C	5:E:175:LEU:H	2.21	0.43
7:G:18:PHE:HA	7:G:22:MET:HE2	2.00	0.43
8:H:118:PHE:C	8:H:120:GLY:N	2.72	0.43
13:T:11:DA:C2	13:T:12:DG:C5	3.06	0.43
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.27	0.43
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.19	0.43
1:A:1341:ILE:C	1:A:1344:GLY:H	2.22	0.43
1:A:1376:THR:O	1:A:1377:THR:C	2.57	0.43
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.43	0.43
1:A:298:PHE:HZ	1:A:314:ALA:HB2	1.82	0.43
1:A:492:PRO:HB3	1:A:501:LEU:CD1	2.49	0.43
1:A:515:GLN:HB2	1:A:1071:SER:HB3	2.00	0.43
1:A:645:LEU:HG	1:A:649:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:THR:CG2	1:A:665:GLY:N	2.81	0.43
1:A:728:LYS:O	1:A:732:LEU:HG	2.19	0.43
1:A:853:ASP:OD1	1:A:855:THR:HB	2.18	0.43
2:B:830:TYR:CZ	2:B:1000:PRO:HB3	2.53	0.43
2:B:401:PHE:HA	2:B:404:LYS:HG3	2.00	0.43
2:B:44:VAL:CG2	2:B:48:LEU:HD11	2.49	0.43
2:B:49:ASP:HA	2:B:52:ASN:HD22	1.84	0.43
2:B:687:GLU:O	2:B:688:GLY:C	2.55	0.43
2:B:811:TYR:N	2:B:811:TYR:HD1	2.13	0.43
2:B:854:LEU:O	2:B:855:PHE:CB	2.63	0.43
2:B:950:ASP:O	2:B:951:GLN:CB	2.66	0.43
3:C:27:LEU:HD11	3:C:178:PHE:CE2	2.54	0.43
3:C:212:PRO:CB	3:C:213:PRO:HD2	2.48	0.43
4:D:120:GLU:HA	4:D:123:LEU:HD12	2.00	0.43
4:D:39:ASN:ND2	4:D:41:GLN:HB2	2.34	0.43
5:E:196:VAL:HG12	5:E:197:LYS:N	2.33	0.43
5:E:151:PRO:HB3	5:E:200:ARG:HB3	2.00	0.43
6:F:105:ALA:HB1	6:F:106:PRO:CD	2.49	0.43
6:F:81:THR:HB	6:F:136:ARG:HH11	1.84	0.43
8:H:40:LEU:HD13	8:H:123:MET:CE	2.48	0.43
8:H:127:GLY:O	8:H:128:ASN:CB	2.66	0.43
9:I:74:GLU:O	9:I:74:GLU:HG3	2.18	0.43
12:L:32:ALA:H	12:L:55:ILE:CG1	2.32	0.43
13:T:12:DG:N2	14:N:6:DT:C2	2.87	0.43
13:T:15:DC:H2"	13:T:16:DT:C6	2.53	0.43
1:A:1213:GLY:HA2	1:A:1216:ILE:HD12	2.01	0.43
1:A:206:GLU:O	1:A:210:ILE:HG13	2.19	0.43
1:A:262:LEU:CD2	1:A:303:TYR:CE1	3.00	0.43
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.48	0.43
1:A:744:LYS:HG2	1:A:748:MET:SD	2.58	0.43
2:B:502:ILE:HG22	2:B:507:LYS:HB2	2.01	0.43
2:B:558:LEU:HD21	2:B:600:LEU:HD11	2.00	0.43
2:B:639:ILE:CD1	2:B:691:GLU:HG3	2.41	0.43
2:B:69:LEU:HD11	2:B:425:THR:HG22	2.00	0.43
2:B:762:ASN:ND2	2:B:1024:ALA:HB3	2.34	0.43
2:B:876:LYS:HD2	2:B:893:LEU:O	2.17	0.43
3:C:269:LYS:O	3:C:270:VAL:HG22	2.18	0.43
4:D:207:LEU:HA	4:D:210:ILE:HD12	2.01	0.43
9:I:13:MET:HG3	9:I:14:LEU:N	2.33	0.43
9:I:68:LEU:HB3	9:I:84:VAL:HG23	2.00	0.43
12:L:44:ASP:O	12:L:45:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:38:LEU:HD11	12:L:49:LYS:HG2	2.01	0.43
1:A:1168:GLU:O	1:A:1172:LEU:HG	2.19	0.43
1:A:1209:MET:O	1:A:1210:GLY:C	2.56	0.43
1:A:1402:PHE:CD1	1:A:1403:GLU:HG3	2.53	0.43
1:A:500:GLU:CD	2:B:1145:SER:HB2	2.39	0.43
2:B:335:GLY:O	2:B:339:THR:HG21	2.19	0.43
2:B:68:THR:CG2	2:B:69:LEU:N	2.82	0.43
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.99	0.43
5:E:198:ILE:HD12	5:E:198:ILE:H	1.83	0.43
1:A:1013:ASP:HB3	5:E:207:ARG:O	2.19	0.43
5:E:46:TYR:CD2	5:E:58:MET:HG2	2.54	0.43
7:G:35:GLU:OE2	7:G:48:VAL:HG23	2.19	0.43
8:H:5:LEU:O	8:H:133:ASN:HB3	2.19	0.43
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.53	0.43
10:J:14:VAL:CG1	10:J:50:ILE:HD11	2.49	0.43
8:H:82:PRO:CG	11:K:54:ARG:HD2	2.46	0.43
1:A:1116:LEU:HA	1:A:1329:THR:HA	2.01	0.43
1:A:1120:LEU:N	1:A:1120:LEU:HD12	2.28	0.43
1:A:1213:GLY:HA2	1:A:1216:ILE:CD1	2.48	0.43
1:A:1434:ALA:HA	1:A:1435:PRO:HD3	1.89	0.43
1:A:244:PRO:CG	1:A:245:PRO:HD3	2.48	0.43
1:A:452:LYS:HG3	2:B:1140:ALA:HB1	1.99	0.43
1:A:489:LEU:HD12	1:A:490:HIS:N	2.33	0.43
1:A:525:GLN:OE1	2:B:836:GLU:HG2	2.19	0.43
1:A:784:LEU:HD11	1:A:815:PHE:CE2	2.54	0.43
1:A:942:PHE:C	1:A:942:PHE:HD2	2.22	0.43
2:B:378:LEU:CD1	2:B:382:ILE:HD11	2.49	0.43
2:B:483:LEU:HD11	2:B:491:THR:CG2	2.49	0.43
2:B:502:ILE:HG22	2:B:507:LYS:HG3	2.01	0.43
2:B:560:GLU:O	2:B:561:TRP:CD1	2.72	0.43
3:C:190:ASP:O	3:C:191:TYR:C	2.57	0.43
3:C:29:MET:HE2	11:K:98:LEU:HD23	2.01	0.43
4:D:60:LYS:NZ	4:D:122:GLU:OE2	2.52	0.43
5:E:89:GLY:C	5:E:91:LYS:H	2.21	0.43
6:F:108:PHE:N	6:F:108:PHE:CD2	2.85	0.43
6:F:93:ILE:HG23	6:F:132:LEU:HD12	2.00	0.43
6:F:82:THR:HA	6:F:83:PRO:HD3	1.66	0.43
9:I:98:VAL:HG12	9:I:99:LEU:H	1.84	0.43
11:K:43:GLY:HA3	11:K:61:TYR:HE1	1.84	0.43
14:N:8:DG:H2"	14:N:9:DA:OP2	2.18	0.43
1:A:1094:VAL:HG12	1:A:1113:THR:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1348:LEU:HD23	1:A:1372:VAL:HG23	2.00	0.43
1:A:153:PRO:HB3	1:A:161:LEU:CD2	2.49	0.43
1:A:254:GLU:O	1:A:255:SER:OG	2.29	0.43
1:A:332:LYS:C	1:A:334:GLY:H	2.22	0.43
1:A:483:ASP:HB2	2:B:987:LYS:CB	2.49	0.43
1:A:541:ILE:HD13	1:A:549:MET:HE1	2.00	0.43
1:A:590:ARG:HG2	1:A:591:PHE:N	2.32	0.43
1:A:57:ARG:O	1:A:68:GLN:HG3	2.19	0.43
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	2.01	0.43
2:B:1181:GLU:H	2:B:1188:LYS:HG3	1.83	0.43
2:B:273:LEU:O	2:B:276:ILE:HB	2.19	0.43
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.45	0.43
2:B:210:LYS:HG3	2:B:461:LEU:O	2.18	0.43
2:B:566:LEU:HD22	2:B:586:TRP:O	2.19	0.43
2:B:864:LYS:HG3	2:B:872:GLU:OE1	2.18	0.43
3:C:229:TYR:CD1	3:C:229:TYR:N	2.87	0.43
4:D:9:GLN:HE22	4:D:31:GLN:HB3	1.84	0.43
5:E:155:ARG:O	5:E:156:LEU:HD23	2.19	0.43
5:E:90:VAL:HG23	5:E:120:ALA:HA	2.01	0.43
6:F:138:LEU:HD22	6:F:139:PRO:HD2	2.00	0.43
6:F:74:ILE:HG22	6:F:75:PRO:N	2.33	0.43
9:I:55:THR:O	9:I:58:VAL:HG23	2.19	0.43
10:J:36:LEU:HD22	10:J:41:LEU:HD12	2.01	0.43
1:A:1341:ILE:CG2	1:A:1342:GLU:H	2.32	0.43
1:A:506:ALA:CB	1:A:508:PRO:HD2	2.49	0.43
1:A:540:PHE:CD1	1:A:540:PHE:N	2.87	0.43
1:A:586:ILE:HD11	1:A:633:VAL:HA	2.00	0.43
1:A:531:ILE:N	1:A:653:VAL:HG11	2.34	0.43
1:A:699:ALA:HB1	9:I:114:GLN:NE2	2.34	0.43
1:A:867:ILE:N	1:A:867:ILE:HD12	2.33	0.43
1:A:886:ILE:HG23	1:A:887:GLY:H	1.80	0.43
1:A:939:ASP:O	1:A:940:ARG:C	2.57	0.43
2:B:603:LEU:HB3	2:B:609:ILE:CD1	2.29	0.43
2:B:700:SER:O	2:B:701:ILE:HG22	2.18	0.43
2:B:816:GLU:OE1	2:B:816:GLU:N	2.49	0.43
3:C:174:ALA:O	3:C:175:ALA:CB	2.67	0.43
3:C:31:ASN:O	3:C:32:SER:C	2.58	0.43
3:C:77:ILE:HA	3:C:129:ILE:HD11	2.01	0.43
4:D:214:LEU:O	4:D:218:GLU:N	2.50	0.43
7:G:114:LEU:HA	7:G:114:LEU:HD12	1.90	0.43
9:I:88:SER:HB3	9:I:95:THR:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:12:LEU:HD23	11:K:16:GLU:O	2.19	0.43
1:A:1202:MET:HE1	1:A:1207:LEU:HB3	2.00	0.42
1:A:123:ARG:O	1:A:124:GLN:C	2.57	0.42
1:A:1303:GLU:HG3	1:A:1303:GLU:O	2.19	0.42
1:A:1453:TYR:O	1:A:1454:MET:HB3	2.19	0.42
1:A:179:LEU:CD1	1:A:297:GLN:HG3	2.49	0.42
1:A:380:VAL:HG13	1:A:385:ILE:CD1	2.48	0.42
1:A:477:PRO:HG2	1:A:521:MET:HG2	2.00	0.42
1:A:730:GLY:O	1:A:731:ARG:C	2.56	0.42
1:A:811:GLN:O	1:A:812:GLU:C	2.57	0.42
2:B:758:PHE:HZ	2:B:1031:LEU:HD22	1.84	0.42
2:B:727:LYS:HE2	2:B:1049:ASP:OD1	2.20	0.42
2:B:1070:GLU:OE1	10:J:44:TYR:OH	2.36	0.42
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.33	0.42
2:B:469:GLN:CG	2:B:470:LYS:N	2.80	0.42
2:B:459:TYR:CE1	2:B:469:GLN:HB3	2.54	0.42
2:B:498:THR:N	2:B:537:LYS:O	2.52	0.42
2:B:731:VAL:HG12	2:B:732:SER:N	2.33	0.42
2:B:35:SER:HA	2:B:811:TYR:HE2	1.84	0.42
2:B:888:GLY:O	2:B:889:THR:C	2.56	0.42
3:C:124:LEU:CD2	3:C:129:ILE:O	2.68	0.42
3:C:24:ASN:CA	3:C:226:ASP:HB3	2.47	0.42
3:C:55:THR:O	3:C:55:THR:HG22	2.19	0.42
4:D:153:ARG:NH2	4:D:184:ALA:HA	2.34	0.42
4:D:219:THR:HG22	4:D:220:LEU:O	2.19	0.42
4:D:39:ASN:ND2	4:D:41:GLN:CG	2.82	0.42
5:E:136:ASN:OD1	5:E:138:ALA:N	2.52	0.42
7:G:38:CYS:HA	7:G:43:GLY:O	2.19	0.42
7:G:62:LEU:CB	7:G:63:PRO:CD	2.91	0.42
8:H:10:PHE:N	8:H:10:PHE:CD1	2.87	0.42
2:B:797:TYR:O	10:J:1:MET:HG2	2.19	0.42
1:A:1100:ARG:O	1:A:1100:ARG:HD2	2.19	0.42
1:A:1135:ARG:C	1:A:1137:ALA:H	2.22	0.42
1:A:1166:ASP:OD2	1:A:1239:ARG:NE	2.45	0.42
1:A:1140:HIS:CA	1:A:1275:GLY:HA3	2.49	0.42
1:A:1376:THR:HG23	1:A:1377:THR:H	1.85	0.42
1:A:293:GLU:O	1:A:295:LEU:N	2.52	0.42
1:A:335:ARG:HA	1:A:339:ASN:ND2	2.32	0.42
1:A:353:ILE:HG13	1:A:353:ILE:O	2.19	0.42
1:A:53:LEU:HD23	1:A:54:ASN:CB	2.46	0.42
1:A:751:SER:O	1:A:752:LYS:CG	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:ILE:HG21	1:A:1374:VAL:HG22	2.02	0.42
1:A:373:THR:HG21	2:B:1105:ALA:HB3	2.00	0.42
2:B:332:ASP:C	2:B:334:ILE:H	2.22	0.42
2:B:351:TYR:CD1	2:B:355:ILE:HD11	2.54	0.42
2:B:654:ARG:C	2:B:656:GLY:N	2.71	0.42
2:B:882:THR:HG21	2:B:935:ARG:CA	2.40	0.42
2:B:891:ASP:C	2:B:893:LEU:N	2.72	0.42
3:C:58:LEU:HD12	3:C:62:PHE:CD1	2.54	0.42
4:D:119:ARG:HG3	4:D:221:TYR:HE2	1.84	0.42
5:E:154:ILE:O	5:E:196:VAL:HA	2.20	0.42
5:E:31:THR:OG1	5:E:34:GLU:N	2.35	0.42
6:F:116:ASP:OD1	6:F:118:LEU:N	2.52	0.42
6:F:75:PRO:C	6:F:77:ASP:N	2.70	0.42
7:G:111:THR:HG22	7:G:113:HIS:H	1.84	0.42
8:H:143:LEU:N	8:H:143:LEU:HD12	2.34	0.42
9:I:86:PHE:HE1	9:I:100:PHE:HB2	1.84	0.42
9:I:55:THR:O	9:I:55:THR:HG22	2.20	0.42
9:I:55:THR:O	9:I:56:ALA:C	2.58	0.42
1:A:12:ARG:HD2	2:B:1218:THR:CG2	2.48	0.42
1:A:1400:CYS:O	1:A:1405:THR:HA	2.19	0.42
1:A:1409:LEU:O	1:A:1412:ALA:HB3	2.19	0.42
1:A:25:GLU:O	1:A:28:ARG:N	2.52	0.42
1:A:705:LYS:O	1:A:706:HIS:C	2.57	0.42
1:A:722:LEU:N	1:A:722:LEU:HD12	2.33	0.42
1:A:781:ASP:HB3	1:A:790:ASP:H	1.83	0.42
1:A:814:PHE:O	1:A:817:ALA:HB3	2.20	0.42
2:B:1065:GLN:HG3	2:B:1067:ARG:N	2.31	0.42
2:B:420:LEU:O	2:B:423:LYS:N	2.48	0.42
2:B:824:ILE:HG12	10:J:48:ARG:HH12	1.84	0.42
2:B:893:LEU:HD22	2:B:897:GLY:O	2.20	0.42
3:C:131:HIS:HA	3:C:132:PRO:HD3	1.76	0.42
3:C:136:ASP:CB	3:C:141:GLY:H	2.32	0.42
3:C:69:LEU:N	3:C:69:LEU:CD1	2.81	0.42
3:C:86:CYS:SG	3:C:87:PHE:N	2.92	0.42
6:F:71:GLU:O	6:F:72:LYS:C	2.57	0.42
6:F:74:ILE:HG22	6:F:75:PRO:O	2.19	0.42
6:F:82:THR:HG23	6:F:83:PRO:HD2	2.01	0.42
7:G:145:VAL:CG1	7:G:146:LYS:N	2.81	0.42
8:H:58:THR:C	8:H:59:ILE:HG13	2.40	0.42
12:L:36:SER:O	12:L:37:LYS:O	2.37	0.42
12:L:58:LYS:O	12:L:59:ALA:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:16:DT:H2"	13:T:17:DT:C5'	2.37	0.42
1:A:1243:VAL:HG22	1:A:1244:ARG:N	2.34	0.42
1:A:1369:ALA:HA	1:A:1372:VAL:HG12	2.01	0.42
1:A:90:VAL:HG13	1:A:297:GLN:HA	2.01	0.42
1:A:38:PRO:CD	1:A:39:GLU:H	2.32	0.42
1:A:398:GLU:O	1:A:399:HIS:C	2.57	0.42
1:A:578:LEU:HD23	1:A:612:ILE:CD1	2.50	0.42
1:A:692:ASP:C	1:A:694:THR:H	2.21	0.42
1:A:709:THR:HG22	1:A:710:LEU:H	1.84	0.42
2:B:828:ALA:HB2	2:B:1085:ILE:HG23	2.02	0.42
2:B:205:ILE:O	2:B:206:ASN:C	2.57	0.42
2:B:298:LEU:N	2:B:298:LEU:CD2	2.82	0.42
2:B:449:ASN:C	2:B:451:LYS:N	2.70	0.42
2:B:700:SER:O	2:B:701:ILE:CG2	2.68	0.42
2:B:880:THR:O	2:B:881:ASN:HB2	2.20	0.42
2:B:955:THR:HG23	2:B:956:THR:N	2.33	0.42
2:B:975:GLN:HG2	2:B:976:ILE:H	1.84	0.42
4:D:208:GLU:O	4:D:209:ARG:C	2.58	0.42
6:F:108:PHE:CE1	6:F:131:PRO:HG3	2.54	0.42
6:F:150:GLU:O	6:F:151:LEU:C	2.57	0.42
1:A:1450:LEU:HD11	7:G:18:PHE:O	2.18	0.42
7:G:1:MET:O	7:G:2:PHE:O	2.36	0.42
7:G:45:ILE:HD13	7:G:78:VAL:HG11	2.01	0.42
1:A:567:LYS:CG	8:H:94:ASP:O	2.64	0.42
14:N:4:DA:H2"	14:N:5:DC:C5	2.54	0.42
2:B:766:ARG:NH2	15:P:11:U:H3	2.17	0.42
1:A:1019:CYS:HA	1:A:1022:LEU:HB3	2.02	0.42
1:A:1054:LEU:HD13	6:F:84:TYR:OH	2.19	0.42
1:A:1121:GLU:O	1:A:1122:PRO:C	2.57	0.42
1:A:1129:GLU:O	1:A:1130:GLN:C	2.57	0.42
1:A:1202:MET:SD	1:A:1207:LEU:HD12	2.60	0.42
1:A:222:LEU:HB3	1:A:223:GLY:H	1.72	0.42
1:A:862:ASN:HA	5:E:174:GLN:HB3	2.01	0.42
1:A:971:PHE:C	1:A:973:ILE:N	2.72	0.42
1:A:96:ILE:HG22	1:A:97:ALA:N	2.34	0.42
2:B:247:GLY:C	2:B:249:ARG:H	2.23	0.42
2:B:510:LYS:HD2	2:B:511:PRO:HD3	2.00	0.42
2:B:593:PRO:CA	2:B:596:LEU:HB3	2.49	0.42
2:B:653:VAL:HG22	2:B:689:LEU:HD13	2.02	0.42
2:B:806:THR:O	2:B:809:MET:HG3	2.20	0.42
2:B:821:GLN:HE22	2:B:851:PHE:CA	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:955:THR:HG23	2:B:956:THR:H	1.84	0.42
3:C:238:ILE:HG12	3:C:246:ARG:NH1	2.35	0.42
4:D:53:SER:HB3	4:D:153:ARG:H	1.84	0.42
4:D:156:ASP:O	4:D:160:VAL:HG23	2.20	0.42
4:D:210:ILE:O	4:D:213:GLU:HB2	2.19	0.42
7:G:153:GLN:HG2	7:G:154:VAL:N	2.34	0.42
7:G:21:ARG:HG2	7:G:24:GLN:HG2	2.02	0.42
7:G:99:PHE:CD1	7:G:99:PHE:O	2.73	0.42
8:H:11:GLN:O	8:H:28:ALA:CB	2.67	0.42
8:H:139:ASN:O	8:H:140:ALA:CB	2.67	0.42
8:H:3:ASN:O	8:H:60:ALA:HB1	2.20	0.42
10:J:16:ASP:O	10:J:18:TRP:N	2.52	0.42
12:L:28:LYS:HD2	12:L:39:SER:OG	2.18	0.42
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.35	0.42
1:A:1152:ILE:HD11	9:I:44:TYR:CD2	2.47	0.42
1:A:1164:PRO:C	1:A:1166:ASP:H	2.23	0.42
1:A:1189:SER:OG	1:A:1256:GLU:OE1	2.32	0.42
1:A:464:PRO:O	1:A:465:TYR:HB2	2.20	0.42
1:A:474:VAL:HG23	1:A:521:MET:HE1	2.02	0.42
1:A:637:LYS:HB3	1:A:641:VAL:CG2	2.33	0.42
1:A:859:SER:HB2	1:A:1422:ARG:HB2	2.01	0.42
1:A:857:ARG:CD	1:A:861:GLY:O	2.60	0.42
1:A:867:ILE:HG12	1:A:1000:LEU:HD11	2.01	0.42
1:A:946:VAL:HG22	5:E:201:LYS:HD2	2.02	0.42
2:B:806:THR:CG2	2:B:1046:PRO:HD3	2.47	0.42
2:B:1110:PRO:HG3	2:B:1125:ASP:HB3	2.01	0.42
2:B:227:LYS:H	2:B:395:GLN:CD	2.23	0.42
2:B:294:ASP:C	2:B:296:GLU:N	2.72	0.42
2:B:459:TYR:CZ	2:B:469:GLN:HB3	2.55	0.42
2:B:46:GLN:NE2	2:B:496:ARG:CB	2.82	0.42
3:C:100:THR:HG21	3:C:102:GLN:NE2	2.35	0.42
3:C:166:GLU:HG3	11:K:10:PHE:HZ	1.84	0.42
4:D:119:ARG:HB2	4:D:221:TYR:CE2	2.53	0.42
4:D:52:LEU:O	4:D:53:SER:OG	2.36	0.42
5:E:78:LEU:CA	5:E:107:THR:HB	2.41	0.42
6:F:70:LYS:C	6:F:72:LYS:N	2.72	0.42
7:G:111:THR:O	7:G:112:LYS:C	2.57	0.42
7:G:51:TYR:C	7:G:51:TYR:CD2	2.93	0.42
7:G:53:ASN:HD22	7:G:53:ASN:N	2.17	0.42
8:H:129:TYR:H	8:H:130:ARG:NH1	2.14	0.42
8:H:5:LEU:HD13	8:H:135:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:50:THR:HG23	9:I:52:ILE:HG12	2.02	0.42
10:J:35:ALA:O	10:J:38:ARG:HB3	2.19	0.42
10:J:42:LYS:HE2	10:J:43:ARG:H	1.85	0.42
2:B:992:ILE:CD1	11:K:66:PRO:HB2	2.49	0.42
11:K:79:GLU:CG	11:K:80:GLY:N	2.82	0.42
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.84	0.42
1:A:1074:GLU:H	1:A:1075:PRO:HD2	1.85	0.42
1:A:1119:TYR:O	1:A:1120:LEU:O	2.38	0.42
1:A:1161:THR:O	1:A:1163:ILE:N	2.53	0.42
1:A:443:LEU:HD22	1:A:443:LEU:HA	1.87	0.42
1:A:640:GLN:HA	1:A:640:GLN:OE1	2.19	0.42
1:A:680:THR:HG23	2:B:729:ILE:HD11	2.01	0.42
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.26	0.42
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.19	0.42
2:B:1116:ARG:HD2	2:B:1198:TYR:CD1	2.55	0.42
2:B:122:LEU:O	2:B:206:ASN:N	2.53	0.42
2:B:257:LYS:N	2:B:270:LYS:O	2.53	0.42
2:B:469:GLN:HG3	2:B:470:LYS:N	2.23	0.42
2:B:653:VAL:HG22	2:B:689:LEU:HB3	2.02	0.42
2:B:969:ARG:HD3	3:C:61:GLU:OE2	2.20	0.42
2:B:831:SER:CB	2:B:994:TYR:OH	2.68	0.42
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.55	0.42
3:C:26:ASP:O	3:C:29:MET:HB3	2.20	0.42
4:D:137:ASN:C	4:D:139:LYS:H	2.23	0.42
5:E:96:PHE:O	5:E:99:HIS:HB3	2.18	0.42
6:F:77:ASP:O	6:F:78:GLN:CB	2.65	0.42
7:G:29:LYS:O	7:G:30:LEU:C	2.58	0.42
9:I:80:SER:OG	9:I:105:SER:CB	2.68	0.42
9:I:76:PRO:HD3	9:I:110:PHE:CD2	2.54	0.42
3:C:3:GLU:HG3	11:K:104:ASN:HD21	1.85	0.42
11:K:79:GLU:C	11:K:81:TYR:H	2.23	0.42
1:A:1115:SER:OG	1:A:1116:LEU:N	2.51	0.42
1:A:1293:SER:HB3	1:A:1297:GLU:O	2.20	0.42
1:A:1114:PRO:O	1:A:1330:ASN:ND2	2.53	0.42
1:A:1438:THR:O	6:F:92:ARG:NH1	2.52	0.42
1:A:1450:LEU:HG	1:A:1450:LEU:O	2.19	0.42
1:A:332:LYS:C	1:A:333:GLU:HG2	2.40	0.42
1:A:370:ILE:CG2	1:A:374:LEU:HG	2.50	0.42
1:A:531:ILE:HD13	1:A:653:VAL:HG21	1.98	0.42
1:A:785:PRO:HG2	1:A:786:HIS:CD2	2.54	0.42
1:A:867:ILE:CG1	1:A:1000:LEU:HD11	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1034:VAL:O	2:B:1036:ALA:N	2.52	0.42
2:B:1065:GLN:NE2	2:B:1066:SER:N	2.67	0.42
1:A:351:THR:HG21	2:B:1103:ILE:HG13	2.01	0.42
2:B:281:PRO:HB3	2:B:320:ASP:OD2	2.18	0.42
2:B:53:GLN:CG	2:B:547:VAL:CG2	2.96	0.42
2:B:642:ASP:CA	2:B:649:LYS:HA	2.27	0.42
2:B:659:ALA:HA	2:B:662:MET:HE2	2.02	0.42
2:B:839:MET:CE	2:B:1010:LEU:HD11	2.50	0.42
3:C:213:PRO:O	3:C:214:ASN:HB3	2.19	0.42
4:D:64:VAL:HG22	4:D:129:LEU:CD2	2.49	0.42
7:G:1:MET:HE1	7:G:3:PHE:HE1	1.85	0.42
9:I:53:GLY:HA2	9:I:56:ALA:HB2	2.02	0.42
2:B:800:GLN:CB	10:J:52:THR:CG2	2.96	0.42
1:A:134:ARG:C	1:A:136:ALA:N	2.73	0.42
1:A:1402:PHE:O	1:A:1403:GLU:CB	2.68	0.42
1:A:115:LEU:CD1	1:A:142:CYS:HB3	2.50	0.42
1:A:444:PHE:HB3	1:A:458:HIS:CD2	2.55	0.42
1:A:528:LEU:HD23	1:A:751:SER:CB	2.45	0.42
1:A:537:ARG:HH22	8:H:122:LEU:CG	2.32	0.42
1:A:896:ARG:HB3	1:A:897:TYR:HD1	1.85	0.42
2:B:1023:VAL:C	2:B:1025:HIS:N	2.73	0.42
2:B:449:ASN:O	2:B:450:ALA:C	2.58	0.42
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.92	0.42
2:B:895:ASP:C	2:B:897:GLY:N	2.73	0.42
3:C:31:ASN:O	3:C:34:ARG:HB3	2.20	0.42
4:D:67:ARG:HA	4:D:133:THR:HG21	2.02	0.42
5:E:156:LEU:HD12	5:E:195:VAL:CG1	2.50	0.42
8:H:4:THR:HG22	8:H:5:LEU:N	2.35	0.42
8:H:98:TYR:HE1	8:H:139:ASN:HA	1.85	0.42
12:L:49:LYS:O	12:L:50:ASP:CB	2.66	0.42
1:A:1277:GLU:O	1:A:1279:ILE:HD12	2.20	0.42
1:A:1314:SER:C	1:A:1315:GLU:HG3	2.40	0.42
1:A:168:GLY:O	1:A:169:ASN:C	2.58	0.42
1:A:362:ASP:O	1:A:458:HIS:HA	2.20	0.42
1:A:391:LEU:O	1:A:394:ASN:HB3	2.20	0.42
1:A:440:ASP:O	1:A:460:VAL:HG23	2.20	0.42
1:A:474:VAL:C	1:A:477:PRO:HD2	2.39	0.42
1:A:456:MET:HE1	1:A:507:VAL:HG13	2.00	0.42
1:A:521:MET:O	1:A:624:SER:HB3	2.20	0.42
1:A:528:LEU:HD11	1:A:619:LYS:H	1.85	0.42
1:A:616:VAL:HG12	1:A:617:VAL:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:ASN:C	1:A:628:GLY:H	2.21	0.42
1:A:62:ASP:O	1:A:62:ASP:OD1	2.38	0.42
1:A:675:THR:HG21	1:A:736:ASN:CG	2.41	0.42
1:A:744:LYS:C	1:A:748:MET:HE2	2.40	0.42
1:A:765:VAL:HG23	1:A:802:ASN:O	2.20	0.42
1:A:885:THR:HG23	1:A:893:PHE:HE1	1.85	0.42
1:A:879:GLU:OE2	1:A:959:ASN:HB2	2.20	0.42
2:B:906:SER:O	2:B:907:GLY:O	2.38	0.42
2:B:956:THR:HG22	2:B:957:ASN:N	2.34	0.42
3:C:16:ASP:O	3:C:17:ASN:CG	2.59	0.42
5:E:134:THR:O	5:E:135:PHE:CD1	2.73	0.42
5:E:13:TRP:O	5:E:16:PHE:N	2.53	0.42
1:A:1017:LEU:HD23	5:E:204:THR:C	2.40	0.42
5:E:207:ARG:NH1	5:E:207:ARG:HB3	2.34	0.42
5:E:16:PHE:CD1	5:E:58:MET:HE2	2.54	0.42
7:G:153:GLN:CG	7:G:154:VAL:HG23	2.43	0.42
8:H:12:VAL:HG13	8:H:26:ILE:CG2	2.50	0.42
8:H:26:ILE:CG2	8:H:27:GLU:H	2.24	0.42
8:H:84:ALA:HA	8:H:87:ARG:HB2	2.01	0.42
9:I:19:ASP:CB	9:I:24:ARG:HG3	2.50	0.42
1:A:1010:ALA:HA	1:A:1013:ASP:OD2	2.20	0.41
1:A:1033:GLN:O	1:A:1036:ARG:NH1	2.53	0.41
1:A:840:ARG:HH22	1:A:1106:ASN:HD21	1.67	0.41
1:A:1191:TRP:HD1	1:A:1256:GLU:CB	2.32	0.41
1:A:293:GLU:C	1:A:295:LEU:N	2.73	0.41
1:A:779:PHE:HD1	1:A:784:LEU:HA	1.85	0.41
1:A:800:VAL:HG11	1:A:808:LEU:HD11	2.02	0.41
1:A:885:THR:O	1:A:885:THR:CG2	2.67	0.41
1:A:898:ARG:HA	1:A:933:TYR:CD1	2.55	0.41
2:B:1177:HIS:O	2:B:1178:ASN:HB2	2.18	0.41
2:B:235:SER:HB3	2:B:258:LEU:HG	2.02	0.41
2:B:44:VAL:HG23	2:B:48:LEU:CD1	2.50	0.41
1:A:315:LEU:CD1	2:B:471:LYS:HB3	2.45	0.41
2:B:980:PHE:HE2	2:B:1094:ARG:CB	2.29	0.41
3:C:67:LEU:HD23	3:C:70:ILE:HD11	2.02	0.41
5:E:167:ARG:HD3	5:E:167:ARG:HA	1.76	0.41
5:E:98:ILE:HG22	5:E:102:GLU:CD	2.41	0.41
6:F:85:MET:HG2	6:F:89:GLU:HB2	2.02	0.41
8:H:108:SER:O	8:H:110:ASP:N	2.53	0.41
1:A:562:THR:HB	8:H:98:TYR:CE2	2.55	0.41
2:B:1100:ASP:OD2	11:K:1:MET:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:GLY:O	1:A:335:ARG:C	2.58	0.41
1:A:41:MET:HE1	1:A:42:ASP:HB2	2.02	0.41
1:A:481:ASP:N	1:A:481:ASP:OD2	2.53	0.41
1:A:636:GLU:OE2	1:A:962:ARG:NH1	2.53	0.41
1:A:745:GLN:HA	1:A:748:MET:CE	2.50	0.41
1:A:838:GLN:O	1:A:841:LEU:HB2	2.20	0.41
2:B:1011:ILE:HG22	2:B:1011:ILE:O	2.19	0.41
2:B:1047:PHE:O	2:B:1048:THR:HG23	2.20	0.41
2:B:1064:TYR:O	2:B:1065:GLN:C	2.59	0.41
2:B:1072:MET:HE3	2:B:1085:ILE:CB	2.41	0.41
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	2.02	0.41
2:B:23:ALA:O	2:B:654:ARG:HB3	2.20	0.41
2:B:610:ASN:C	2:B:612:GLU:H	2.23	0.41
2:B:664:THR:CG2	2:B:678:GLU:N	2.83	0.41
2:B:781:PHE:O	2:B:782:LEU:HG	2.20	0.41
3:C:124:LEU:HD21	3:C:129:ILE:O	2.20	0.41
3:C:213:PRO:O	3:C:214:ASN:CB	2.68	0.41
3:C:269:LYS:HD3	3:C:270:VAL:HG13	2.01	0.41
4:D:53:SER:OG	4:D:54:GLU:N	2.52	0.41
4:D:68:ARG:C	4:D:70:PHE:H	2.22	0.41
1:A:537:ARG:NH1	8:H:122:LEU:HG	2.34	0.41
9:I:2:THR:O	9:I:3:THR:C	2.58	0.41
9:I:61:ASP:C	9:I:63:GLY:H	2.23	0.41
10:J:6:ARG:HB3	10:J:11:GLY:O	2.20	0.41
11:K:13:GLY:O	11:K:14:GLU:O	2.38	0.41
13:T:12:DG:H2''	13:T:13:DT:O5'	2.20	0.41
1:A:1107:VAL:HG21	1:A:1383:SER:HB3	2.02	0.41
1:A:1330:ASN:O	1:A:1332:PHE:N	2.53	0.41
1:A:134:ARG:C	1:A:136:ALA:H	2.23	0.41
1:A:705:LYS:HB2	1:A:708:MET:CE	2.49	0.41
1:A:767:GLN:NE2	1:A:797:LYS:O	2.53	0.41
1:A:846:GLU:OE1	1:A:1425:SER:OG	2.38	0.41
1:A:910:PRO:HB3	1:A:917:SER:N	2.29	0.41
1:A:894:GLU:HG2	1:A:933:TYR:OH	2.21	0.41
1:A:946:VAL:HG13	5:E:201:LYS:CB	2.38	0.41
2:B:26:THR:HA	2:B:708:GLU:OE1	2.20	0.41
2:B:886:LYS:HB3	2:B:887:HIS:H	1.73	0.41
2:B:982:SER:HB3	2:B:1092:TYR:CE2	2.55	0.41
2:B:1001:PHE:HD2	3:C:34:ARG:HH21	1.64	0.41
5:E:52:ARG:CG	5:E:52:ARG:NH1	2.81	0.41
5:E:89:GLY:HA2	5:E:117:THR:OG1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:116:ASP:OD1	6:F:119:ARG:N	2.54	0.41
8:H:24:CYS:HB2	8:H:44:VAL:CG2	2.48	0.41
8:H:41:ASP:O	8:H:42:ILE:CB	2.67	0.41
1:A:1037:LEU:HD13	1:A:1041:ALA:CB	2.50	0.41
1:A:1276:VAL:CG1	1:A:1277:GLU:H	2.29	0.41
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.21	0.41
1:A:1444:MET:O	6:F:133:VAL:N	2.53	0.41
1:A:377:PRO:HD2	1:A:493:GLN:OE1	2.20	0.41
1:A:516:SER:O	1:A:518:LYS:HB3	2.20	0.41
1:A:543:LEU:HD12	1:A:547:LEU:HG	2.03	0.41
1:A:92:HIS:O	1:A:94:GLY:N	2.53	0.41
1:A:343:LYS:HB3	2:B:1117:GLN:OE1	2.21	0.41
2:B:1183:LYS:C	2:B:1185:CYS:N	2.73	0.41
2:B:344:LYS:O	2:B:345:LYS:C	2.59	0.41
2:B:355:ILE:H	2:B:355:ILE:HG13	1.71	0.41
2:B:593:PRO:CG	2:B:617:ARG:NH2	2.83	0.41
2:B:685:LEU:HG	2:B:686:ASN:N	2.33	0.41
2:B:745:PRO:C	2:B:747:MET:N	2.72	0.41
2:B:868:MET:O	2:B:870:ILE:HG13	2.19	0.41
4:D:155:ARG:NH1	4:D:155:ARG:CG	2.84	0.41
4:D:2:ASN:O	4:D:4:SER:N	2.44	0.41
6:F:90:ARG:HG2	6:F:155:LEU:HD13	2.02	0.41
7:G:20:PRO:CG	7:G:21:ARG:H	2.33	0.41
8:H:63:LEU:CD1	8:H:64:ASN:N	2.84	0.41
2:B:619:ILE:CG2	9:I:61:ASP:HB2	2.51	0.41
12:L:27:LEU:HB2	12:L:28:LYS:H	1.78	0.41
1:A:1035:TYR:O	1:A:1036:ARG:C	2.58	0.41
1:A:1317:MET:C	1:A:1319:VAL:H	2.24	0.41
1:A:1446:ASP:O	1:A:1447:GLU:C	2.58	0.41
1:A:188:ASP:O	1:A:195:ASP:HA	2.20	0.41
1:A:218:ASP:O	1:A:219:PHE:C	2.59	0.41
1:A:483:ASP:HB2	2:B:987:LYS:HB3	2.01	0.41
1:A:614:PHE:CB	8:H:122:LEU:HD21	2.50	0.41
1:A:865:GLN:OE1	1:A:869:GLY:N	2.44	0.41
1:A:930:ASP:O	1:A:931:GLU:C	2.58	0.41
2:B:1074:ASN:O	2:B:1076:HIS:N	2.53	0.41
1:A:1431:GLY:HA3	2:B:1197:PRO:HD3	2.02	0.41
2:B:343:ILE:HG23	2:B:347:LYS:HE2	2.01	0.41
2:B:744:HIS:CG	2:B:745:PRO:HD2	2.55	0.41
2:B:119:LEU:HD22	2:B:789:MET:HB2	2.02	0.41
2:B:795:ILE:HD12	2:B:795:ILE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:880:THR:HB	2:B:934:LYS:CD	2.39	0.41
2:B:893:LEU:C	2:B:894:ASP:O	2.58	0.41
2:B:957:ASN:O	2:B:958:GLN:C	2.58	0.41
3:C:209:TYR:H	3:C:209:TYR:HD1	1.69	0.41
6:F:118:LEU:O	6:F:122:MET:CG	2.68	0.41
6:F:73:ALA:CB	6:F:143:PHE:H	2.34	0.41
12:L:53:HIS:C	12:L:55:ILE:HD13	2.41	0.41
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	2.01	0.41
1:A:1420:ASP:O	1:A:1421:CYS:CB	2.64	0.41
1:A:455:MET:HE3	2:B:1134:GLU:HG3	2.02	0.41
1:A:441:PRO:HG3	1:A:498:ARG:HB2	2.02	0.41
1:A:552:TRP:HE3	1:A:651:LYS:HB3	1.85	0.41
1:A:58:LEU:O	1:A:59:GLY:O	2.39	0.41
1:A:622:VAL:HG22	1:A:622:VAL:O	2.20	0.41
1:A:523:ILE:CD1	1:A:649:ILE:HG21	2.51	0.41
1:A:870:GLU:O	1:A:871:ASP:HB3	2.19	0.41
1:A:874:ASP:C	1:A:874:ASP:OD1	2.59	0.41
2:B:1003:ALA:O	3:C:177:GLU:HG2	2.21	0.41
2:B:116:GLU:C	2:B:118:ARG:H	2.24	0.41
1:A:16:GLU:CG	2:B:1220:ARG:HA	2.51	0.41
2:B:255:GLN:O	2:B:271:ALA:HB1	2.20	0.41
2:B:278:GLN:HG2	2:B:279:ASP:N	2.35	0.41
2:B:303:TYR:HH	2:B:586:TRP:HH2	1.65	0.41
2:B:705:MET:HE1	2:B:742:GLU:HG2	2.02	0.41
4:D:130:LEU:C	4:D:132:GLN:N	2.73	0.41
4:D:153:ARG:HD3	4:D:154:PHE:CE1	2.54	0.41
5:E:205:SER:O	5:E:206:GLY:C	2.59	0.41
8:H:77:ARG:O	8:H:78:SER:O	2.38	0.41
9:I:35:VAL:CG1	9:I:36:GLU:N	2.79	0.41
11:K:98:LEU:O	11:K:99:GLY:C	2.59	0.41
1:A:967:ALA:HA	1:A:1044:TRP:CZ3	2.56	0.41
1:A:874:ASP:N	1:A:1058:VAL:HG23	2.36	0.41
1:A:1118:VAL:HG23	1:A:1118:VAL:O	2.20	0.41
1:A:1230:GLU:C	1:A:1232:ASN:H	2.23	0.41
1:A:1135:ARG:HB2	1:A:1306:LEU:HD11	2.02	0.41
1:A:1434:ALA:O	1:A:1436:ILE:N	2.53	0.41
1:A:515:GLN:HB2	1:A:1071:SER:CB	2.51	0.41
1:A:567:LYS:HG2	1:A:568:PRO:CD	2.51	0.41
2:B:224:GLN:O	2:B:238:ALA:HA	2.20	0.41
2:B:467:GLY:N	2:B:475:SER:HB3	2.35	0.41
2:B:51:PHE:O	2:B:54:PHE:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:582:VAL:O	2:B:582:VAL:HG12	2.21	0.41
2:B:656:GLY:O	2:B:657:HIS:C	2.59	0.41
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.55	0.41
2:B:766:ARG:HH11	2:B:766:ARG:CG	2.31	0.41
3:C:99:LEU:HA	3:C:119:VAL:O	2.20	0.41
3:C:43:THR:CG2	3:C:44:LEU:N	2.60	0.41
4:D:176:GLU:HG2	4:D:197:SER:OG	2.20	0.41
5:E:112:TYR:CZ	5:E:136:ASN:HB2	2.55	0.41
5:E:112:TYR:HE1	5:E:136:ASN:HD22	1.68	0.41
5:E:14:ARG:HB3	5:E:141:VAL:O	2.19	0.41
5:E:159:ASP:O	5:E:160:GLU:C	2.59	0.41
5:E:172:GLU:O	5:E:175:LEU:HB2	2.21	0.41
5:E:165:LEU:HD21	5:E:175:LEU:HD11	2.03	0.41
5:E:190:LEU:HA	5:E:190:LEU:HD22	1.84	0.41
5:E:164:LEU:HD11	5:E:211:TYR:CE1	2.56	0.41
6:F:109:VAL:CG2	6:F:124:GLU:HG2	2.50	0.41
6:F:89:GLU:OE2	6:F:134:ILE:HG21	2.20	0.41
8:H:128:ASN:O	8:H:128:ASN:OD1	2.38	0.41
8:H:89:LEU:HB2	8:H:91:ASP:OD1	2.21	0.41
9:I:61:ASP:O	9:I:63:GLY:N	2.54	0.41
2:B:797:TYR:O	10:J:1:MET:CG	2.69	0.41
1:A:1301:GLU:O	1:A:1302:PRO:O	2.39	0.41
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.65	0.41
1:A:565:ILE:HD13	8:H:46:LEU:HD12	2.03	0.41
1:A:635:ARG:HH21	1:A:877:HIS:HA	1.84	0.41
1:A:913:LEU:HD21	1:A:915:SER:OG	2.20	0.41
1:A:921:GLY:O	1:A:922:ASP:C	2.58	0.41
2:B:1020:ARG:HG3	2:B:1020:ARG:NH1	2.34	0.41
2:B:705:MET:HE3	2:B:742:GLU:HB2	2.02	0.41
2:B:840:ILE:HB	2:B:1011:ILE:HB	2.02	0.41
2:B:120:ARG:CD	2:B:955:THR:HG21	2.50	0.41
3:C:221:TYR:CD1	3:C:222:LYS:HG3	2.55	0.41
3:C:20:PHE:HE2	3:C:232:VAL:HG23	1.86	0.41
3:C:79:GLN:HG3	3:C:127:ARG:HD2	2.03	0.41
4:D:130:LEU:CD1	4:D:142:LYS:HG3	2.51	0.41
4:D:71:LYS:HA	4:D:74:GLN:HB2	2.02	0.41
1:A:1342:GLU:CD	5:E:198:ILE:HG21	2.41	0.41
5:E:38:PRO:HG2	5:E:41:ASP:OD2	2.21	0.41
5:E:94:LYS:HE2	5:E:98:ILE:HD11	2.02	0.41
6:F:96:THR:O	6:F:99:LEU:HB3	2.21	0.41
9:I:111:THR:CG2	9:I:112:SER:H	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:29:CYS:SG	9:I:31:THR:HB	2.61	0.41
10:J:14:VAL:CG1	10:J:14:VAL:O	2.68	0.41
10:J:44:TYR:HD2	10:J:44:TYR:N	2.03	0.41
10:J:56:LEU:HB3	10:J:60:PHE:CE2	2.55	0.41
1:A:1006:ILE:HD12	5:E:167:ARG:HB2	2.03	0.41
1:A:1026:LEU:HD23	1:A:1026:LEU:HA	1.72	0.41
1:A:1094:VAL:O	1:A:1095:THR:C	2.60	0.41
1:A:1224:LEU:HD12	1:A:1241:ARG:O	2.21	0.41
1:A:1276:VAL:CG1	1:A:1277:GLU:N	2.82	0.41
1:A:319:GLY:O	1:A:320:ARG:C	2.60	0.41
1:A:360:GLU:C	1:A:471:ASN:HD22	2.24	0.41
1:A:427:GLN:HB2	1:A:430:TRP:NE1	2.35	0.41
1:A:434:ARG:NH1	1:A:434:ARG:HG2	2.33	0.41
1:A:371:ALA:HB2	1:A:462:VAL:HG13	2.03	0.41
1:A:944:ARG:CZ	1:A:1298:TYR:CE1	3.04	0.41
1:A:919:ILE:HD13	1:A:983:ILE:HD12	2.03	0.41
2:B:999:MET:HG2	2:B:1007:VAL:CG2	2.50	0.41
2:B:1041:GLU:O	2:B:1042:GLY:C	2.59	0.41
2:B:306:ASN:C	2:B:308:TRP:N	2.74	0.41
2:B:326:ASP:OD1	2:B:329:THR:N	2.47	0.41
2:B:332:ASP:OD1	2:B:348:ARG:CZ	2.69	0.41
2:B:334:ILE:HB	2:B:352:ALA:HB2	2.02	0.41
2:B:571:PRO:HG2	2:B:572:HIS:CE1	2.56	0.41
2:B:620:ARG:NH2	9:I:86:PHE:CD2	2.89	0.41
2:B:686:ASN:C	2:B:688:GLY:N	2.74	0.41
2:B:918:ILE:HD12	2:B:935:ARG:NH1	2.35	0.41
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.21	0.41
2:B:999:MET:HB3	2:B:1007:VAL:HG21	2.03	0.41
6:F:85:MET:HB3	6:F:155:LEU:HD11	2.02	0.41
7:G:20:PRO:HG2	7:G:21:ARG:N	2.36	0.41
9:I:94:ASP:O	9:I:95:THR:O	2.38	0.41
11:K:40:HIS:O	11:K:41:THR:C	2.59	0.41
12:L:29:TYR:HA	12:L:57:LEU:O	2.20	0.41
1:A:1139:GLU:O	1:A:1140:HIS:C	2.60	0.41
1:A:298:PHE:O	1:A:301:ALA:HB3	2.21	0.41
1:A:349:ALA:C	2:B:1128:LEU:HD11	2.41	0.41
1:A:351:THR:CG2	2:B:1103:ILE:HG13	2.51	0.41
1:A:383:TYR:HD2	1:A:383:TYR:N	2.15	0.41
1:A:535:THR:HG23	1:A:575:LYS:HG2	2.02	0.41
1:A:600:PRO:HG2	1:A:601:LYS:HG3	2.03	0.41
1:A:741:ASN:HD22	1:A:744:LYS:N	2.14	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:ILE:CG2	1:A:887:GLY:H	2.34	0.41
1:A:897:TYR:H	1:A:897:TYR:HD1	1.67	0.41
2:B:114:PRO:O	2:B:116:GLU:N	2.54	0.41
2:B:1169:MET:O	2:B:1170:THR:C	2.58	0.41
2:B:221:ASN:HA	2:B:241:ARG:O	2.21	0.41
2:B:311:LEU:O	2:B:314:LEU:N	2.54	0.41
2:B:323:VAL:HG12	2:B:323:VAL:O	2.20	0.41
2:B:619:ILE:HD13	9:I:64:SER:OG	2.21	0.41
3:C:101:LEU:HD13	3:C:118:LEU:CD2	2.31	0.41
5:E:74:ASP:N	5:E:74:ASP:OD1	2.50	0.41
6:F:75:PRO:C	6:F:77:ASP:H	2.24	0.41
6:F:90:ARG:CG	6:F:91:ALA:N	2.81	0.41
7:G:114:LEU:HD23	7:G:161:GLY:O	2.20	0.41
1:A:614:PHE:HB2	8:H:122:LEU:HD21	2.02	0.41
8:H:32:THR:CG2	8:H:33:GLN:N	2.80	0.41
9:I:82:GLU:HB3	9:I:104:LEU:CG	2.50	0.41
10:J:2:ILE:HG23	10:J:3:VAL:H	1.85	0.41
11:K:51:LEU:HD13	11:K:59:ALA:HB3	2.03	0.41
1:A:112:LYS:HG2	1:A:113:LEU:N	2.36	0.41
1:A:1224:LEU:HG	1:A:1226:VAL:HG23	2.02	0.41
1:A:1225:PHE:HZ	1:A:1227:ILE:HD11	1.85	0.41
1:A:227:VAL:O	1:A:228:PHE:HD2	2.04	0.41
1:A:416:ARG:NH1	1:A:417:TYR:HE2	2.19	0.41
1:A:355:GLY:HA3	1:A:482:PHE:CZ	2.56	0.41
1:A:574:GLY:O	1:A:575:LYS:C	2.59	0.41
1:A:783:THR:HG21	1:A:815:PHE:CE2	2.56	0.41
2:B:1060:ARG:NE	3:C:202:PRO:HG3	2.36	0.41
2:B:98:THR:O	2:B:126:SER:CB	2.69	0.41
1:A:825:ILE:HD13	2:B:512:ARG:HB3	2.00	0.41
1:A:818:MET:N	2:B:514:LEU:HD23	2.35	0.41
2:B:662:MET:HA	2:B:665:GLU:HB2	2.03	0.41
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.87	0.41
2:B:785:TYR:CE2	10:J:60:PHE:CE1	3.08	0.41
2:B:843:GLN:NE2	2:B:847:ASP:OD1	2.52	0.41
2:B:911:ILE:HG23	2:B:966:VAL:HG11	2.02	0.41
4:D:189:ASP:O	4:D:193:THR:CB	2.69	0.41
4:D:53:SER:O	4:D:57:LEU:HG	2.21	0.41
6:F:113:GLY:O	6:F:114:GLU:C	2.59	0.41
6:F:118:LEU:O	6:F:122:MET:HG3	2.20	0.41
8:H:82:PRO:HG2	8:H:83:GLN:H	1.86	0.41
10:J:45:CYS:O	10:J:48:ARG:NE	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:7:PHE:HA	11:K:10:PHE:HE2	1.86	0.41
1:A:1191:TRP:HD1	1:A:1256:GLU:HB3	1.86	0.40
1:A:130:ASP:O	1:A:132:LYS:N	2.54	0.40
1:A:1444:MET:HE2	1:A:1444:MET:HB2	1.91	0.40
1:A:317:LYS:HG2	2:B:471:LYS:HZ1	1.85	0.40
1:A:497:THR:O	1:A:500:GLU:HB2	2.21	0.40
1:A:584:ASN:HA	1:A:609:ASP:O	2.22	0.40
1:A:630:ILE:CD1	1:A:646:PHE:HZ	2.31	0.40
1:A:68:GLN:C	1:A:70:CYS:N	2.72	0.40
2:B:1102:LYS:CA	2:B:1122:ARG:NH1	2.84	0.40
2:B:345:LYS:C	2:B:348:ARG:HG2	2.42	0.40
2:B:56:ASP:HB2	2:B:57:TYR:CD1	2.56	0.40
2:B:684:LEU:O	2:B:689:LEU:HB2	2.21	0.40
2:B:863:GLU:O	2:B:961:LEU:HD22	2.21	0.40
4:D:123:LEU:HG	4:D:149:THR:CG2	2.51	0.40
4:D:57:LEU:CD1	4:D:160:VAL:HG21	2.44	0.40
6:F:117:PRO:HG2	6:F:118:LEU:H	1.86	0.40
9:I:1:MET:HE2	9:I:4:PHE:HB3	2.03	0.40
3:C:3:GLU:CG	11:K:104:ASN:HD21	2.33	0.40
11:K:68:PHE:N	11:K:68:PHE:CD2	2.89	0.40
1:A:1050:GLU:HG3	1:A:1051:ALA:N	2.35	0.40
1:A:1127:ASP:OD1	1:A:1130:GLN:HB2	2.20	0.40
1:A:1170:ILE:HG22	1:A:1174:PHE:CE1	2.57	0.40
1:A:335:ARG:HE	1:A:335:ARG:HA	1.85	0.40
1:A:40:THR:CB	1:A:41:MET:HE2	2.49	0.40
1:A:51:GLY:HA2	1:A:56:PRO:HA	2.03	0.40
1:A:596:THR:C	1:A:597:LEU:HD12	2.41	0.40
1:A:605:MET:HG2	1:A:621:THR:CG2	2.51	0.40
1:A:804:TYR:HE1	2:B:1021:MET:HE3	1.85	0.40
1:A:953:ASN:C	1:A:954:TRP:CD1	2.95	0.40
1:A:982:THR:C	1:A:984:LYS:N	2.75	0.40
1:A:335:ARG:NH1	2:B:1202:LEU:CD2	2.79	0.40
2:B:258:LEU:O	2:B:259:TYR:O	2.39	0.40
1:A:814:PHE:CD1	2:B:519:TRP:HE3	2.39	0.40
2:B:782:LEU:HD12	2:B:788:ARG:HH11	1.86	0.40
2:B:901:PRO:HA	2:B:949:VAL:HG12	2.03	0.40
5:E:207:ARG:CB	5:E:207:ARG:NH1	2.84	0.40
8:H:135:LEU:HD13	8:H:137:GLN:HE21	1.81	0.40
9:I:7:CYS:CB	9:I:14:LEU:HD21	2.31	0.40
3:C:114:TYR:HE2	10:J:19:GLU:OE2	2.05	0.40
12:L:32:ALA:HB2	12:L:55:ILE:CG1	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1192:LEU:HD13	1:A:1239:ARG:NH1	2.36	0.40
1:A:320:ARG:HA	1:A:321:PRO:HD3	1.94	0.40
1:A:33:ALA:O	1:A:83:HIS:CD2	2.74	0.40
1:A:672:ASP:O	1:A:673:GLY:C	2.59	0.40
1:A:73:GLY:O	1:A:74:MET:C	2.60	0.40
1:A:91:PHE:HB3	1:A:96:ILE:CG1	2.51	0.40
2:B:1146:PHE:O	2:B:1147:LEU:C	2.60	0.40
2:B:50:SER:OG	2:B:411:PRO:HD3	2.21	0.40
2:B:640:VAL:O	2:B:640:VAL:HG12	2.21	0.40
2:B:658:ILE:HG22	2:B:662:MET:CE	2.49	0.40
2:B:749:LEU:HB3	2:B:753:ALA:HB3	2.02	0.40
2:B:497:ARG:HH12	2:B:775:LYS:HE2	1.86	0.40
2:B:785:TYR:CD2	2:B:785:TYR:N	2.89	0.40
2:B:944:THR:HG21	2:B:1122:ARG:CZ	2.48	0.40
3:C:112:ASN:N	3:C:112:ASN:HD22	2.19	0.40
3:C:54:ASN:HB2	3:C:153:LEU:HD12	2.02	0.40
4:D:56:ARG:HA	4:D:148:LEU:HD13	2.02	0.40
4:D:187:THR:C	4:D:189:ASP:N	2.75	0.40
4:D:189:ASP:O	4:D:193:THR:HB	2.20	0.40
4:D:31:GLN:C	4:D:33:PHE:H	2.23	0.40
4:D:75:LYS:HB3	4:D:75:LYS:HE2	1.92	0.40
5:E:161:LYS:O	5:E:164:LEU:N	2.54	0.40
5:E:190:LEU:HD13	5:E:191:LYS:H	1.87	0.40
5:E:32:GLN:HG3	5:E:36:GLU:OE2	2.22	0.40
7:G:127:PRO:CB	7:G:139:ILE:HD11	2.51	0.40
9:I:68:LEU:HB3	9:I:84:VAL:CG2	2.52	0.40
11:K:6:ARG:HA	11:K:6:ARG:HD3	1.90	0.40
1:A:1067:LEU:HD12	1:A:1367:HIS:CE1	2.57	0.40
1:A:230:ARG:N	1:A:233:TRP:HE3	2.11	0.40
1:A:284:ALA:O	1:A:286:HIS:N	2.47	0.40
1:A:269:ILE:CG2	1:A:300:VAL:HG22	2.51	0.40
1:A:334:GLY:O	1:A:336:ILE:N	2.55	0.40
1:A:356:ASP:OD2	11:K:65:HIS:CE1	2.70	0.40
1:A:438:ASP:O	1:A:439:ASN:CB	2.64	0.40
1:A:473:SER:OG	1:A:646:PHE:HD2	2.04	0.40
1:A:546:VAL:HG21	1:A:572:TRP:CE3	2.57	0.40
1:A:556:TRP:C	1:A:558:GLY:N	2.74	0.40
1:A:608:ILE:CB	1:A:613:ILE:HD11	2.48	0.40
1:A:688:LYS:HA	1:A:691:LEU:HB3	2.03	0.40
1:A:72:GLU:CB	1:A:76:GLU:HG2	2.48	0.40
1:A:873:MET:C	1:A:1058:VAL:CG2	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:PRO:HB2	1:A:875:ALA:HB3	2.04	0.40
2:B:1135:ARG:HG3	2:B:1147:LEU:HD11	2.03	0.40
1:A:78:PRO:CB	2:B:1201:LYS:HE3	2.49	0.40
2:B:276:ILE:HG22	2:B:278:GLN:O	2.21	0.40
2:B:293:PRO:C	2:B:294:ASP:O	2.58	0.40
2:B:349:ILE:O	2:B:353:LYS:HG3	2.22	0.40
2:B:582:VAL:CG2	2:B:626:ILE:HB	2.51	0.40
2:B:903:VAL:HG12	2:B:904:ARG:N	2.37	0.40
3:C:183:TRP:O	3:C:184:ASN:C	2.59	0.40
3:C:233:GLU:O	3:C:240:VAL:HG13	2.22	0.40
3:C:242:GLN:O	3:C:244:VAL:N	2.54	0.40
4:D:7:THR:HG21	4:D:32:GLU:OE2	2.20	0.40
8:H:138:GLU:O	8:H:139:ASN:C	2.58	0.40
11:K:28:PRO:O	11:K:29:ASN:C	2.58	0.40
12:L:47:ARG:NH1	12:L:47:ARG:HG3	2.36	0.40
1:A:1277:GLU:C	1:A:1279:ILE:H	2.25	0.40
1:A:341:MET:CE	1:A:843:LYS:HZ2	2.35	0.40
1:A:417:TYR:O	1:A:418:SER:C	2.60	0.40
1:A:418:SER:C	1:A:420:ARG:N	2.72	0.40
1:A:481:ASP:OD1	1:A:483:ASP:OD1	2.39	0.40
1:A:565:ILE:HG22	1:A:565:ILE:O	2.22	0.40
1:A:590:ARG:HD2	1:A:605:MET:HB2	2.04	0.40
1:A:720:ARG:NH1	1:A:720:ARG:HB2	2.36	0.40
1:A:734:GLU:C	1:A:736:ASN:N	2.74	0.40
1:A:77:CYS:C	1:A:78:PRO:O	2.59	0.40
1:A:833:GLU:HG3	1:A:1102:LYS:HZ1	1.86	0.40
1:A:977:LYS:HB3	1:A:978:PRO:HD2	2.03	0.40
2:B:1006:ILE:HD13	10:J:44:TYR:CZ	2.56	0.40
2:B:1197:PRO:C	2:B:1199:ALA:N	2.74	0.40
2:B:95:ILE:HA	2:B:129:PHE:O	2.22	0.40
2:B:167:ILE:CD1	2:B:167:ILE:N	2.82	0.40
2:B:170:LEU:HD12	2:B:171:PRO:N	2.37	0.40
2:B:195:CYS:HB2	2:B:784:ASN:OD1	2.22	0.40
2:B:253:THR:CG2	2:B:254:LEU:H	2.28	0.40
2:B:326:ASP:OD1	2:B:328:GLU:HB3	2.21	0.40
2:B:167:ILE:CG2	2:B:453:ILE:HD12	2.40	0.40
2:B:467:GLY:O	2:B:468:GLU:C	2.59	0.40
2:B:705:MET:HB3	2:B:706:GLN:H	1.70	0.40
2:B:791:THR:HG22	2:B:858:SER:HB2	2.04	0.40
2:B:797:TYR:HE1	2:B:971:THR:HG23	1.87	0.40
2:B:834:ASN:HB3	2:B:840:ILE:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:131:HIS:O	3:C:133:ILE:N	2.54	0.40
2:B:995:ARG:NH1	3:C:165:LYS:HG2	2.37	0.40
4:D:130:LEU:HA	4:D:134:THR:OG1	2.22	0.40
4:D:39:ASN:HD21	4:D:41:GLN:CG	2.33	0.40
5:E:153:HIS:C	5:E:154:ILE:HG13	2.42	0.40
5:E:173:SER:C	5:E:175:LEU:N	2.75	0.40
1:A:1342:GLU:OE2	5:E:212:ARG:NH1	2.55	0.40
10:J:7:CYS:CB	10:J:49:MET:HE3	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1421/1733 (82%)	929 (65%)	311 (22%)	181 (13%)	0	5
2	B	1111/1224 (91%)	712 (64%)	251 (23%)	148 (13%)	0	4
3	C	268/324 (83%)	165 (62%)	69 (26%)	34 (13%)	0	5
4	D	178/221 (80%)	125 (70%)	29 (16%)	24 (14%)	0	4
5	E	212/215 (99%)	145 (68%)	42 (20%)	25 (12%)	0	6
6	F	86/155 (56%)	60 (70%)	21 (24%)	5 (6%)	1	21
7	G	169/171 (99%)	133 (79%)	25 (15%)	11 (6%)	1	19
8	H	133/146 (91%)	78 (59%)	26 (20%)	29 (22%)	0	1
9	I	115/122 (94%)	72 (63%)	29 (25%)	14 (12%)	0	6
10	J	63/70 (90%)	35 (56%)	14 (22%)	14 (22%)	0	1
11	K	114/120 (95%)	80 (70%)	31 (27%)	3 (3%)	5	35
12	L	45/70 (64%)	18 (40%)	13 (29%)	14 (31%)	0	0
All	All	3915/4571 (86%)	2552 (65%)	861 (22%)	502 (13%)	0	5

All (502) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	41	MET
1	A	43	GLU
1	A	48	ALA
1	A	54	ASN
1	A	58	LEU
1	A	67	CYS
1	A	69	THR
1	A	73	GLY
1	A	76	GLU
1	A	84	ILE
1	A	130	ASP
1	A	154	SER
1	A	167	CYS
1	A	187	LYS
1	A	193	ASP
1	A	259	GLU
1	A	311	GLN
1	A	312	PRO
1	A	317	LYS
1	A	318	SER
1	A	385	ILE
1	A	410	GLY
1	A	439	ASN
1	A	536	LEU
1	A	567	LYS
1	A	583	PRO
1	A	603	ASN
1	A	641	VAL
1	A	666	ILE
1	A	775	ILE
1	A	846	GLU
1	A	852	TYR
1	A	875	ALA
1	A	916	GLY
1	A	968	GLN
1	A	973	ILE
1	A	1002	GLY
1	A	1016	THR
1	A	1036	ARG
1	A	1114	PRO
1	A	1115	SER

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Mol	Chain	Res	Type
1	A	1116	LEU
1	A	1120	LEU
1	A	1122	PRO
1	A	1167	GLU
1	A	1176	LEU
1	A	1177	LEU
1	A	1178	ASP
1	A	1202	MET
1	A	1212	VAL
1	A	1223	ASP
1	A	1233	ASP
1	A	1244	ARG
1	A	1255	GLU
1	A	1314	SER
1	A	1341	ILE
1	A	1361	SER
1	A	1365	TYR
1	A	1378	GLN
2	B	46	GLN
2	B	68	THR
2	B	108	VAL
2	B	124	TYR
2	B	186	GLU
2	B	229	ALA
2	B	282	ILE
2	B	344	LYS
2	B	345	LYS
2	B	346	GLU
2	B	365	THR
2	B	367	LEU
2	B	391	ASP
2	B	468	GLU
2	B	469	GLN
2	B	509	ALA
2	B	511	PRO
2	B	543	SER
2	B	566	LEU
2	B	575	PRO
2	B	629	ASP
2	B	705	MET
2	B	707	PRO
2	B	708	GLU

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Mol	Chain	Res	Type
2	B	712	PRO
2	B	723	VAL
2	B	751	VAL
2	B	855	PHE
2	B	867	GLY
2	B	879	ARG
2	B	882	THR
2	B	907	GLY
2	B	958	GLN
2	B	1041	GLU
2	B	1045	SER
2	B	1046	PRO
2	B	1069	PHE
2	B	1097	HIS
2	B	1156	ASP
2	B	1171	VAL
2	B	1175	LEU
2	B	1181	GLU
2	B	1183	LYS
3	C	6	PRO
3	C	56	THR
3	C	60	ASP
3	C	77	ILE
3	C	90	ASP
3	C	110	THR
3	C	133	ILE
3	C	141	GLY
3	C	149	LYS
3	C	161	LYS
3	C	173	ALA
3	C	174	ALA
3	C	175	ALA
3	C	215	GLU
3	C	216	GLY
3	C	237	SER
3	C	269	LYS
4	D	3	VAL
4	D	12	ARG
4	D	19	GLU
4	D	52	LEU
4	D	169	SER
5	E	43	LYS

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Mol	Chain	Res	Type
5	E	45	LYS
5	E	73	PRO
5	E	106	GLN
5	E	115	ASN
5	E	129	PRO
5	E	130	ALA
5	E	174	GLN
5	E	192	ARG
5	E	206	GLY
6	F	71	GLU
6	F	72	LYS
6	F	81	THR
6	F	139	PRO
7	G	2	PHE
7	G	120	THR
7	G	139	ILE
7	G	154	VAL
8	H	42	ILE
8	H	78	SER
8	H	84	ALA
8	H	87	ARG
8	H	92	ASP
8	H	128	ASN
8	H	131	ASN
8	H	140	ALA
9	I	8	ARG
9	I	11	ASN
9	I	79	HIS
9	I	95	THR
9	I	106	CYS
10	J	2	ILE
10	J	64	ASN
11	K	14	GLU
11	K	79	GLU
12	L	40	LEU
12	L	42	ARG
12	L	50	ASP
12	L	55	ILE
12	L	59	ALA
12	L	60	ARG
1	A	57	ARG
1	A	70	CYS

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Mol	Chain	Res	Type
1	A	74	MET
1	A	93	VAL
1	A	96	ILE
1	A	131	SER
1	A	148	CYS
1	A	281	HIS
1	A	283	GLY
1	A	313	GLN
1	A	332	LYS
1	A	399	HIS
1	A	419	LYS
1	A	556	TRP
1	A	591	PHE
1	A	600	PRO
1	A	619	LYS
1	A	706	HIS
1	A	719	VAL
1	A	752	LYS
1	A	780	VAL
1	A	789	LYS
1	A	871	ASP
1	A	922	ASP
1	A	969	GLN
1	A	972	HIS
1	A	1050	GLU
1	A	1064	VAL
1	A	1140	HIS
1	A	1206	ASP
1	A	1221	LYS
1	A	1279	ILE
1	A	1302	PRO
1	A	1316	VAL
1	A	1393	ASN
1	A	1437	GLY
2	B	21	GLU
2	B	45	SER
2	B	48	LEU
2	B	56	ASP
2	B	65	GLU
2	B	134	LYS
2	B	135	ARG
2	B	257	LYS

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Mol	Chain	Res	Type
2	B	259	TYR
2	B	277	LYS
2	B	278	GLN
2	B	312	GLU
2	B	327	ARG
2	B	341	LEU
2	B	364	ILE
2	B	450	ALA
2	B	470	LYS
2	B	483	LEU
2	B	506	GLY
2	B	512	ARG
2	B	577	ALA
2	B	709	ASP
2	B	727	LYS
2	B	752	ALA
2	B	754	SER
2	B	894	ASP
2	B	943	SER
2	B	951	GLN
2	B	956	THR
2	B	1075	GLY
2	B	1099	VAL
2	B	1100	ASP
2	B	1131	GLY
2	B	1167	GLY
2	B	1184	GLY
2	B	1223	ASP
3	C	61	GLU
3	C	78	GLU
3	C	128	ASN
3	C	240	VAL
4	D	20	GLU
4	D	47	LEU
4	D	119	ARG
4	D	131	GLU
4	D	192	LYS
4	D	218	GLU
4	D	220	LEU
5	E	3	GLN
5	E	76	GLY
5	E	97	VAL

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Mol	Chain	Res	Type
5	E	121	MET
6	F	150	GLU
7	G	63	PRO
7	G	64	THR
7	G	114	LEU
8	H	18	GLY
8	H	63	LEU
8	H	81	PRO
8	H	82	PRO
8	H	90	ALA
8	H	119	GLY
8	H	137	GLN
9	I	2	THR
9	I	3	THR
9	I	32	CYS
9	I	56	ALA
10	J	17	LYS
10	J	24	LEU
10	J	32	GLU
11	K	15	GLY
12	L	28	LYS
12	L	37	LYS
12	L	53	HIS
12	L	56	LEU
1	A	5	GLN
1	A	38	PRO
1	A	42	ASP
1	A	77	CYS
1	A	86	LEU
1	A	128	ILE
1	A	222	LEU
1	A	232	GLU
1	A	287	HIS
1	A	423	ASP
1	A	424	ILE
1	A	568	PRO
1	A	601	LYS
1	A	604	GLY
1	A	661	GLY
1	A	847	ASP
1	A	885	THR
1	A	979	SER

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Mol	Chain	Res	Type
1	A	1067	LEU
1	A	1105	LEU
1	A	1124	HIS
1	A	1127	ASP
1	A	1165	GLU
1	A	1229	SER
1	A	1331	SER
1	A	1405	THR
1	A	1450	LEU
2	B	37	PHE
2	B	100	PRO
2	B	184	ALA
2	B	265	SER
2	B	295	GLY
2	B	304	ASP
2	B	333	PHE
2	B	343	ILE
2	B	368	GLU
2	B	409	ALA
2	B	559	SER
2	B	591	ARG
2	B	711	GLU
2	B	746	SER
2	B	815	ARG
2	B	848	ARG
2	B	878	GLN
2	B	892	LYS
2	B	909	ASP
2	B	1003	ALA
2	B	1035	ALA
2	B	1082	MET
2	B	1126	GLY
2	B	1155	SER
2	B	1157	ALA
2	B	1176	ASN
3	C	132	PRO
3	C	142	VAL
3	C	213	PRO
4	D	21	GLU
4	D	25	ALA
4	D	32	GLU
4	D	59	ILE

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Mol	Chain	Res	Type
4	D	139	LYS
4	D	168	LYS
4	D	198	LEU
4	D	199	ASN
5	E	48	ASP
5	E	74	ASP
5	E	93	MET
5	E	104	ASN
5	E	173	SER
7	G	141	SER
8	H	2	SER
8	H	107	VAL
8	H	108	SER
8	H	109	LYS
8	H	110	ASP
9	I	47	GLU
10	J	6	ARG
10	J	18	TRP
1	A	55	ASP
1	A	59	GLY
1	A	63	ARG
1	A	126	LEU
1	A	164	ARG
1	A	190	ALA
1	A	196	GLU
1	A	257	ARG
1	A	286	HIS
1	A	300	VAL
1	A	322	VAL
1	A	330	LYS
1	A	409	SER
1	A	525	GLN
1	A	535	THR
1	A	557	ASP
1	A	592	ASP
1	A	738	LYS
1	A	765	VAL
1	A	854	ASN
1	A	1005	GLU
1	A	1068	ALA
1	A	1240	CYS
1	A	1242	VAL

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Mol	Chain	Res	Type
1	A	1366	ARG
1	A	1377	THR
1	A	1399	ARG
1	A	1402	PHE
2	B	41	LYS
2	B	115	GLN
2	B	131	ASP
2	B	267	ARG
2	B	531	GLN
2	B	642	ASP
2	B	688	GLY
2	B	699	GLU
2	B	868	MET
2	B	881	ASN
2	B	891	ASP
2	B	1017	ILE
3	C	108	GLU
3	C	191	TYR
3	C	214	ASN
4	D	4	SER
4	D	13	ARG
4	D	118	THR
5	E	122	LYS
5	E	179	GLN
7	G	118	ASP
8	H	17	PRO
8	H	41	ASP
8	H	52	GLN
8	H	83	GLN
9	I	93	LYS
9	I	107	SER
10	J	9	SER
10	J	14	VAL
10	J	33	GLY
12	L	35	SER
1	A	35	ILE
1	A	52	GLY
1	A	113	LEU
1	A	234	MET
1	A	294	SER
1	A	917	SER
1	A	958	VAL

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Mol	Chain	Res	Type
1	A	986	ILE
1	A	1006	ILE
1	A	1133	LEU
1	A	1211	GLN
2	B	24	PRO
2	B	49	ASP
2	B	171	PRO
2	B	283	VAL
2	B	311	LEU
2	B	456	GLY
2	B	480	SER
2	B	510	LYS
2	B	579	ARG
2	B	594	ALA
2	B	643	ASP
2	B	655	LYS
2	B	793	ALA
2	B	1042	GLY
3	C	11	ARG
4	D	191	ALA
5	E	56	LYS
5	E	148	GLU
7	G	20	PRO
8	H	21	ASN
8	H	132	LEU
10	J	13	VAL
10	J	42	LYS
12	L	36	SER
12	L	46	VAL
1	A	24	PRO
1	A	170	THR
1	A	314	ALA
1	A	517	ASN
1	A	652	VAL
1	A	704	ALA
1	A	818	MET
1	A	845	LEU
1	A	1454	MET
2	B	67	SER
2	B	219	ALA
2	B	903	VAL
2	B	1080	LYS

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Mol	Chain	Res	Type
2	B	1214	PRO
3	C	3	GLU
3	C	36	VAL
3	C	89	GLU
3	C	218	PRO
10	J	55	ASP
12	L	25	ALA
1	A	231	PRO
1	A	244	PRO
1	A	910	PRO
2	B	436	VAL
2	B	478	GLY
2	B	503	GLY
3	C	25	VAL
8	H	120	GLY
1	A	258	GLY
2	B	315	LYS
2	B	780	VAL
9	I	62	ILE
1	A	250	ILE
2	B	305	VAL
2	B	636	PRO
2	B	744	HIS
5	E	86	PRO
7	G	92	VAL
9	I	57	GLY
10	J	57	ILE
1	A	51	GLY
1	A	197	PRO
1	A	718	VAL
1	A	1162	VAL
2	B	114	PRO
2	B	464	GLY
2	B	658	ILE
5	E	53	PRO
8	H	12	VAL
1	A	78	PRO
2	B	334	ILE
3	C	10	ILE
8	H	44	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1249/1520 (82%)	1126 (90%)	123 (10%)	8	31
2	B	974/1061 (92%)	888 (91%)	86 (9%)	10	37
3	C	238/280 (85%)	219 (92%)	19 (8%)	12	41
4	D	164/200 (82%)	145 (88%)	19 (12%)	5	26
5	E	196/197 (100%)	182 (93%)	14 (7%)	14	44
6	F	78/137 (57%)	70 (90%)	8 (10%)	7	30
7	G	152/152 (100%)	144 (95%)	8 (5%)	22	52
8	H	121/128 (94%)	111 (92%)	10 (8%)	11	39
9	I	111/116 (96%)	102 (92%)	9 (8%)	11	40
10	J	60/65 (92%)	55 (92%)	5 (8%)	11	39
11	K	99/102 (97%)	89 (90%)	10 (10%)	7	30
12	L	41/57 (72%)	34 (83%)	7 (17%)	2	14
All	All	3483/4015 (87%)	3165 (91%)	318 (9%)	9	35

All (318) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	34	LYS
1	A	37	PHE
1	A	38	PRO
1	A	41	MET
1	A	54	ASN
1	A	70	CYS
1	A	83	HIS
1	A	85	ASP
1	A	93	VAL
1	A	157	ASP
1	A	185	TRP
1	A	200	ARG
1	A	236	LEU

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Mol	Chain	Res	Type
1	A	245	PRO
1	A	262	LEU
1	A	265	LYS
1	A	275	SER
1	A	307	ASP
1	A	312	PRO
1	A	320	ARG
1	A	322	VAL
1	A	326	ARG
1	A	332	LYS
1	A	335	ARG
1	A	352	VAL
1	A	379	VAL
1	A	385	ILE
1	A	406	ILE
1	A	408	ASP
1	A	412	ARG
1	A	438	ASP
1	A	442	VAL
1	A	443	LEU
1	A	445	ASN
1	A	449	SER
1	A	450	LEU
1	A	451	HIS
1	A	453	MET
1	A	454	SER
1	A	466	SER
1	A	489	LEU
1	A	493	GLN
1	A	503	GLN
1	A	511	ILE
1	A	518	LYS
1	A	540	PHE
1	A	542	GLU
1	A	552	TRP
1	A	557	ASP
1	A	590	ARG
1	A	618	GLU
1	A	634	THR
1	A	635	ARG
1	A	711	ARG
1	A	720	ARG

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Mol	Chain	Res	Type
1	A	727	ASP
1	A	740	LEU
1	A	774	ARG
1	A	779	PHE
1	A	821	ARG
1	A	833	GLU
1	A	842	VAL
1	A	858	ASN
1	A	871	ASP
1	A	903	ASN
1	A	918	GLU
1	A	920	LEU
1	A	929	LEU
1	A	940	ARG
1	A	942	PHE
1	A	947	PHE
1	A	948	VAL
1	A	949	ASP
1	A	976	THR
1	A	995	GLU
1	A	1001	ARG
1	A	1017	LEU
1	A	1019	CYS
1	A	1029	ARG
1	A	1035	TYR
1	A	1037	LEU
1	A	1067	LEU
1	A	1077	THR
1	A	1111	MET
1	A	1120	LEU
1	A	1122	PRO
1	A	1124	HIS
1	A	1128	GLN
1	A	1166	ASP
1	A	1170	ILE
1	A	1178	ASP
1	A	1206	ASP
1	A	1233	ASP
1	A	1239	ARG
1	A	1240	CYS
1	A	1245	PRO
1	A	1255	GLU

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Mol	Chain	Res	Type
1	A	1257	ASP
1	A	1259	MET
1	A	1260	LEU
1	A	1264	GLU
1	A	1280	GLU
1	A	1288	ASP
1	A	1295	THR
1	A	1297	GLU
1	A	1300	LYS
1	A	1308	THR
1	A	1314	SER
1	A	1332	PHE
1	A	1333	ILE
1	A	1336	MET
1	A	1359	ASP
1	A	1364	ASN
1	A	1366	ARG
1	A	1389	PHE
1	A	1391	ARG
1	A	1393	ASN
1	A	1394	THR
1	A	1400	CYS
1	A	1443	VAL
1	A	1445	ILE
1	A	1454	MET
2	B	20	ASP
2	B	31	TRP
2	B	57	TYR
2	B	61	ASP
2	B	100	PRO
2	B	164	LYS
2	B	166	PHE
2	B	167	ILE
2	B	169	ARG
2	B	175	ARG
2	B	180	TYR
2	B	194	GLU
2	B	203	PHE
2	B	217	ARG
2	B	268	THR
2	B	272	THR
2	B	332	ASP

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Mol	Chain	Res	Type
2	B	364	ILE
2	B	365	THR
2	B	371	GLU
2	B	378	LEU
2	B	393	LYS
2	B	396	ASP
2	B	429	PHE
2	B	465	ASN
2	B	466	TRP
2	B	473	MET
2	B	485	ARG
2	B	502	ILE
2	B	510	LYS
2	B	516	ASN
2	B	555	ILE
2	B	563	MET
2	B	572	HIS
2	B	582	VAL
2	B	591	ARG
2	B	603	LEU
2	B	609	ILE
2	B	615	MET
2	B	616	ILE
2	B	636	PRO
2	B	680	THR
2	B	694	ASP
2	B	737	THR
2	B	742	GLU
2	B	743	ILE
2	B	776	GLN
2	B	785	TYR
2	B	790	ASP
2	B	811	TYR
2	B	830	TYR
2	B	839	MET
2	B	854	LEU
2	B	860	MET
2	B	868	MET
2	B	878	GLN
2	B	879	ARG
2	B	894	ASP
2	B	895	ASP

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Mol	Chain	Res	Type
2	B	909	ASP
2	B	918	ILE
2	B	944	THR
2	B	978	ASP
2	B	999	MET
2	B	1046	PRO
2	B	1047	PHE
2	B	1069	PHE
2	B	1076	HIS
2	B	1077	THR
2	B	1084	GLN
2	B	1087	PHE
2	B	1095	LEU
2	B	1097	HIS
2	B	1098	MET
2	B	1103	ILE
2	B	1113	VAL
2	B	1150	ARG
2	B	1151	LEU
2	B	1159	ARG
2	B	1163	CYS
2	B	1170	THR
2	B	1182	CYS
2	B	1189	ILE
2	B	1218	THR
2	B	1221	SER
2	B	1223	ASP
3	C	1	MET
3	C	35	ARG
3	C	38	ILE
3	C	56	THR
3	C	58	LEU
3	C	62	PHE
3	C	77	ILE
3	C	91	HIS
3	C	104	PHE
3	C	106	GLU
3	C	138	GLU
3	C	147	LEU
3	C	166	GLU
3	C	193	TYR
3	C	209	TYR

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Mol	Chain	Res	Type
3	C	226	ASP
3	C	233	GLU
3	C	235	VAL
3	C	250	THR
4	D	8	PHE
4	D	13	ARG
4	D	15	LEU
4	D	21	GLU
4	D	22	GLU
4	D	40	HIS
4	D	47	LEU
4	D	63	LEU
4	D	70	PHE
4	D	118	THR
4	D	127	ASP
4	D	137	ASN
4	D	148	LEU
4	D	149	THR
4	D	189	ASP
4	D	211	LEU
4	D	214	LEU
4	D	215	SER
4	D	221	TYR
5	E	17	ARG
5	E	31	THR
5	E	52	ARG
5	E	60	PHE
5	E	74	ASP
5	E	96	PHE
5	E	104	ASN
5	E	114	ASN
5	E	132	ILE
5	E	149	LEU
5	E	169	ARG
5	E	173	SER
5	E	178	ILE
5	E	190	LEU
6	F	71	GLU
6	F	72	LYS
6	F	79	ARG
6	F	99	LEU
6	F	116	ASP

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Mol	Chain	Res	Type
6	F	118	LEU
6	F	148	VAL
6	F	151	LEU
7	G	1	MET
7	G	13	LEU
7	G	21	ARG
7	G	52	ASP
7	G	73	LYS
7	G	74	TYR
7	G	79	PHE
7	G	94	CYS
8	H	17	PRO
8	H	42	ILE
8	H	63	LEU
8	H	64	ASN
8	H	86	ASP
8	H	88	SER
8	H	89	LEU
8	H	95	TYR
8	H	102	TYR
8	H	110	ASP
9	I	4	PHE
9	I	6	PHE
9	I	7	CYS
9	I	8	ARG
9	I	85	PHE
9	I	86	PHE
9	I	94	ASP
9	I	100	PHE
9	I	101	PHE
10	J	23	ASN
10	J	43	ARG
10	J	44	TYR
10	J	46	CYS
10	J	48	ARG
11	K	5	ASP
11	K	6	ARG
11	K	10	PHE
11	K	25	THR
11	K	47	ARG
11	K	50	LEU
11	K	61	TYR

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Mol	Chain	Res	Type
11	K	81	TYR
11	K	111	LEU
11	K	114	LEU
12	L	27	LEU
12	L	34	CYS
12	L	54	ARG
12	L	55	ILE
12	L	65	VAL
12	L	68	GLU
12	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	83	HIS
1	A	92	HIS
1	A	109	HIS
1	A	169	ASN
1	A	225	ASN
1	A	256	GLN
1	A	299	HIS
1	A	306	ASN
1	A	339	ASN
1	A	358	ASN
1	A	399	HIS
1	A	435	HIS
1	A	445	ASN
1	A	447	GLN
1	A	493	GLN
1	A	603	ASN
1	A	659	HIS
1	A	700	ASN
1	A	736	ASN
1	A	741	ASN
1	A	757	ASN
1	A	767	GLN
1	A	768	GLN
1	A	786	HIS
1	A	851	HIS
1	A	858	ASN
1	A	903	ASN

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Mol	Chain	Res	Type
1	A	926	GLN
1	A	935	GLN
1	A	968	GLN
1	A	975	HIS
1	A	1106	ASN
1	A	1130	GLN
1	A	1140	HIS
1	A	1188	GLN
1	A	1203	ASN
1	A	1278	ASN
1	A	1312	ASN
1	A	1364	ASN
1	A	1393	ASN
1	A	1427	ASN
1	A	1432	GLN
2	B	46	GLN
2	B	60	GLN
2	B	178	ASN
2	B	224	GLN
2	B	236	HIS
2	B	366	GLN
2	B	465	ASN
2	B	484	ASN
2	B	499	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	587	HIS
2	B	686	ASN
2	B	706	GLN
2	B	744	HIS
2	B	763	GLN
2	B	786	ASN
2	B	821	GLN
2	B	842	ASN
2	B	862	GLN
2	B	951	GLN
2	B	975	GLN
2	B	1015	HIS
2	B	1065	GLN
2	B	1076	HIS

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Mol	Chain	Res	Type
2	B	1084	GLN
2	B	1117	GLN
2	B	1178	ASN
2	B	1179	GLN
2	B	1193	GLN
3	C	24	ASN
3	C	65	HIS
3	C	73	GLN
3	C	79	GLN
3	C	102	GLN
3	C	112	ASN
3	C	140	ASN
3	C	167	HIS
3	C	252	GLN
4	D	2	ASN
4	D	9	GLN
4	D	31	GLN
4	D	39	ASN
4	D	40	HIS
4	D	74	GLN
4	D	137	ASN
4	D	138	ASN
4	D	143	ASN
5	E	32	GLN
5	E	99	HIS
5	E	101	GLN
5	E	104	ASN
5	E	114	ASN
5	E	147	HIS
6	F	100	GLN
7	G	53	ASN
7	G	122	ASN
7	G	126	ASN
8	H	33	GLN
8	H	131	ASN
8	H	137	GLN
9	I	12	ASN
9	I	89	GLN
9	I	90	GLN
9	I	108	HIS
9	I	114	GLN
10	J	64	ASN

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Mol	Chain	Res	Type
11	K	29	ASN
11	K	44	ASN
11	K	52	ASN
11	K	65	HIS
11	K	76	GLN
11	K	104	ASN
11	K	110	ASN
12	L	53	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/16 (56%)	2 (22%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	10	A
15	P	11	U

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	8OG	T	19	13,15	18,25,26	1.30	2 (11%)	21,37,40	2.57	5 (23%)
13	BRU	T	23	13,15	15,21,22	4.01	4 (26%)	17,30,33	4.22	5 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	8OG	T	19	13,15	-	2/3/21/22	0/3/3/3
13	BRU	T	23	13,15	-	0/4/21/22	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	23	BRU	BR-C5	-14.14	1.49	1.90
13	T	23	BRU	C4-C5	5.38	1.45	1.38
13	T	19	8OG	C6-N1	3.83	1.39	1.33
13	T	19	8OG	C8-N7	-3.11	1.30	1.34
13	T	23	BRU	C4-N3	2.64	1.37	1.33
13	T	23	BRU	C6-C5	-2.04	1.35	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	23	BRU	C4-N3-C2	15.08	127.87	115.14
13	T	19	8OG	C5-C6-N1	-8.63	111.62	123.43
13	T	23	BRU	C5-C4-N3	-7.08	115.16	123.64
13	T	19	8OG	C6-N1-C2	5.84	125.21	115.93
13	T	19	8OG	C2-N3-C4	-2.86	112.08	115.36
13	T	23	BRU	C5-C6-N1	2.77	123.56	119.97
13	T	19	8OG	N3-C2-N1	-2.52	123.86	127.22
13	T	23	BRU	BR-C5-C6	2.47	122.93	117.31
13	T	19	8OG	C6-C5-C4	-2.37	118.53	120.80
13	T	23	BRU	O3'-C3'-C2'	-2.17	103.15	110.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	T	19	8OG	O4'-C4'-C5'-O5'
13	T	19	8OG	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T	19	8OG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T	23	BRU	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1429/1733 (82%)	-0.21	3 (0%) 95 93	73, 132, 187, 200	0
2	B	1125/1224 (91%)	-0.05	15 (1%) 77 68	79, 146, 196, 200	0
3	C	270/324 (83%)	-0.21	1 (0%) 92 87	92, 133, 183, 200	0
4	D	182/221 (82%)	-0.18	3 (1%) 72 62	122, 160, 195, 200	0
5	E	214/215 (99%)	-0.21	1 (0%) 91 85	111, 170, 198, 200	0
6	F	88/155 (56%)	-0.26	0 100 100	77, 110, 145, 175	0
7	G	171/171 (100%)	-0.16	0 100 100	113, 140, 176, 182	0
8	H	137/146 (93%)	0.28	7 (5%) 28 23	147, 178, 198, 200	0
9	I	117/122 (95%)	-0.01	4 (3%) 45 35	126, 178, 197, 200	0
10	J	65/70 (92%)	-0.30	0 100 100	112, 129, 171, 180	0
11	K	116/120 (96%)	-0.23	2 (1%) 70 60	96, 135, 160, 199	0
12	L	47/70 (67%)	-0.14	0 100 100	128, 169, 190, 200	0
13	T	18/26 (69%)	0.30	0 100 100	182, 200, 200, 200	0
14	N	11/12 (91%)	0.80	0 100 100	196, 200, 200, 200	0
15	P	10/16 (62%)	-0.14	0 100 100	199, 200, 200, 200	0
All	All	4000/4625 (86%)	-0.14	36 (0%) 84 77	73, 142, 196, 200	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	471	LYS	7.2
2	B	504	ARG	4.0
9	I	1	MET	3.9
4	D	76	LYS	3.5
8	H	140	ALA	3.4
2	B	503	GLY	3.3
2	B	722	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	883	LEU	3.1
2	B	470	LYS	3.0
11	K	116	ALA	2.9
8	H	142	LEU	2.9
2	B	505	ASP	2.8
2	B	468	GLU	2.8
2	B	507	LYS	2.7
11	K	115	ALA	2.6
2	B	341	LEU	2.6
8	H	146	ARG	2.5
2	B	339	THR	2.5
8	H	84	ALA	2.4
4	D	1	MET	2.3
8	H	83	GLN	2.3
2	B	723	VAL	2.3
2	B	865	LYS	2.3
2	B	724	ASP	2.2
8	H	143	LEU	2.2
9	I	102	VAL	2.2
3	C	2	SER	2.2
4	D	2	ASN	2.1
1	A	145	LYS	2.1
1	A	1150	SER	2.1
8	H	61	SER	2.1
9	I	84	VAL	2.1
1	A	1455	PRO	2.1
5	E	82	PHE	2.0
2	B	866	TYR	2.0
9	I	26	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
13	BRU	T	23	20/21	0.71	0.23	198,199,200,200	0
13	8OG	T	19	23/24	0.91	0.17	186,193,198,199	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
16	MG	A	2458	1/1	0.93	0.09	200,200,200,200	0
17	ZN	I	1122	1/1	0.95	0.05	198,198,198,198	0
17	ZN	A	2456	1/1	0.97	0.06	150,150,150,150	0
17	ZN	J	1066	1/1	0.99	0.27	135,135,135,135	0
17	ZN	L	1071	1/1	0.99	0.08	158,158,158,158	0
17	ZN	B	2225	1/1	0.99	0.22	106,106,106,106	0
17	ZN	A	2457	1/1	0.99	0.15	107,107,107,107	0
17	ZN	C	1269	1/1	1.00	0.14	101,101,101,101	0
17	ZN	I	1121	1/1	1.00	0.12	140,140,140,140	0

6.5 Other polymers [i](#)

There are no such residues in this entry.